



STIC Search Report

Biotech-Chem Library

STIC Database Tracking Number: 127

TO: Hector Reyes
Location: REM-5C18
Art Unit: 1625
Wednesday, July 21, 2004

Case Serial Number: 10/075442

From: Deirdre Arnold
Location: Biotech-Chem Library
REM 1A64
Phone: 571-272-2532

Deirdre.Arnold@uspto.gov

Search Notes

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Biotech-Chem Library

Questions about the scope or the results of the search? Contact *the searcher or contact*

Mary Hale, Information Branch Supervisor
571-272-2507 Remsen E01 D86

Voluntary Results Feedback Form

✓ I am an examiner in Workgroup: Example: 1610

✓ Relevant prior art **found**, search results used as follows:

- 102 rejection
- 103 rejection
- Cited as being of interest.
- Helped examiner better understand the invention.
- Helped examiner better understand the state of the art in their technology field.

Types of relevant prior art found:

- Foreign Patent(s)
- Non-Patent Literature
(journal articles, conference proceedings, new product announcements etc.)

✓ Relevant prior art **not found**:

- Results verified the lack of relevant prior art (helped determine patentability)
- Results were not useful in determining patentability or understanding the inventive concept.

Comments:

Drop off or send completed forms to STIC/BioTech-Chem Library Remsen Bldg



FILE 'HCAPLUS' ENTERED AT 09:06:29 ON 21 JUL 2004
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FILE COVERS 1907 - 21 Jul 2004 VOL 141 ISS 4
 FILE LAST UPDATED: 20 Jul 2004 (20040720/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> act rey442hcaapp/a
 L24 1 SEA FILE=HCAPLUS ABB=ON PLU=ON US2002-075442/AP, PRN

=> d que 124
 L24 1 SEA FILE=HCAPLUS ABB=ON PLU=ON US2002-075442/AP, PRN

=> d 124 iall

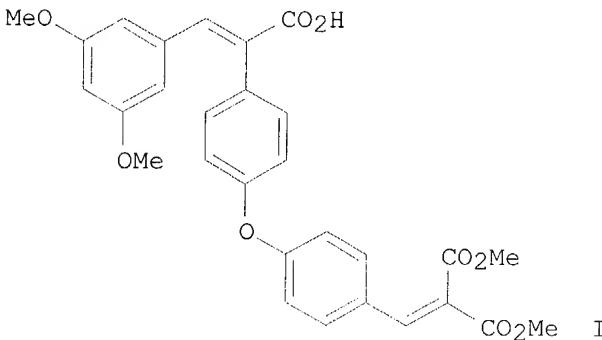
L24 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2001:359750 HCAPLUS
 DOCUMENT NUMBER: 134:348284
 ENTRY DATE: Entered STN: 18 May 2001
 TITLE: Phenyl compounds to treat diabetes and associated conditions
 INVENTOR(S): Neogi, Partha; Nag, Bishwajit; Lakner, Frederick J.;
 Dey, Debendranath; Medicherla, Satyanarayana
 PATENT ASSIGNEE(S): Calyx Therapeutics, Inc., USA
 SOURCE: PCT Int. Appl., 47 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 INT. PATENT CLASSIF.:
 MAIN: A61K
 CLASSIFICATION: 1-10 (Pharmacology)
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

*Saint
 Inverness*

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001034094	A2	20010517	WO 2000-US30927	20001108
WO 2001034094	C2	20020725		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,			

LU, LV, MA, MD, MG, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
 SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
 YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
 US 6525093 B1 20030225 US 1999-436047 19991108
 AU 2001017607 A5 20010606 AU 2001-17607 20001108
 EP 1235785 A2 20020904 EP 2000-980331 20001108
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
 JP 2004503464 T2 20040205 JP 2001-536099 20001108
 US 2002107285 A1 20020808 US 2002-75442 20020215 <--
 PRIORITY APPLN. INFO.: US 1999-436047 A 19991108
 WO 2000-US30927 W 20001108

OTHER SOURCE(S): MARPAT 134:348284
 GRAPHIC IMAGE:



ABSTRACT:

Ph compds. (Markush included) are provided that lower blood glucose concns., lower serum triglyceride concns., lower systolic blood pressure, and increase glucose uptake by adipose tissue, but do not affect the expression of PPAR- γ by adipose tissue. Compds. of the invention include e.g. I.

SUPPL. TERM: phenyl deriv antidiabetic hypotriglyceridemic
 antihypertensive

INDEX TERM: Antidiabetic agents
 Antihypertensives
 Drug delivery systems
 Hypolipemic agents
 (Ph compds. to treat diabetes and associated conditions)

INDEX TERM: Glycerides, biological studies
 ROLE: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
 (blood; Ph compds. to treat diabetes and associated conditions)

INDEX TERM: Peroxisome proliferator-activated receptors
 ROLE: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
 (γ ; Ph compds. to treat diabetes and associated conditions)

INDEX TERM: 339332-56-8 339332-57-9
 ROLE: BAC (Biological activity or effector, except adverse);

BSU (Biological study, unclassified); THU (Therapeutic use);
BIOL (Biological study); USES (Uses)

INDEX TERM: (Ph compds. to treat diabetes and associated conditions)
50-99-7, D-Glucose, biological studies

ROLE: BPR (Biological process); BSU (Biological study,
unclassified); BIOL (Biological study); PROC (Process)

(Ph compds. to treat diabetes and associated conditions)

=> FIL STNGUIDE

4/4

Reyes 10/075,442

07/21/2004

=> fil zcaplus

FILE 'ZCPLUS' ENTERED AT 08:36:01 ON 21 JUL 2004
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=> fil biosis

FILE 'BIOSIS' ENTERED AT 08:36:06 ON 21 JUL 2004
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FILE COVERS 1969 TO DATE.
CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT
FROM JANUARY 1969 TO DATE.

RECORDS LAST ADDED: 15 July 2004 (20040715/ED)

FILE RELOADED: 19 October 2003.

=> FIL STNGUIDE

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FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Jul 16, 2004 (20040716/UP).

=> d que l10

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L1 ( 114) SEA FILE=HCAPLUS ABB=ON PLU=ON ("NEOGI P"/AU OR "NEOGI P K
      B"/AU OR "NEOGI P S"/AU) OR ("NEOGI PARTHA"/AU OR "NEOGI
      PARTHASAKHA"/AU)
L2 ( 287) SEA FILE=HCAPLUS ABB=ON NAG/AU OR ("NAG B"/AU OR "NAG
      B B"/AU OR "NAG B B S P"/AU OR "NAG B D"/AU OR "NAG B D
      CHOWDHURI"/AU OR "NAG B L"/AU OR "NAG B N"/AU OR "NAG B R"/AU)
      OR ("NAG BISHWAGIT"/AU OR "NAG BISHWAJIT"/AU)
L3 ( 17) SEA FILE=HCAPLUS ABB=ON PLU=ON ("LAKNER F J"/AU OR "LAKNER
      FREDERICK J"/AU OR "LAKNER FREDERICK JAMES"/AU OR "LAKNER
      FREDRICK J"/AU)
L4 ( 21) SEA FILE=HCAPLUS ABB=ON PLU=ON ("DEV D"/AU OR "DEV D K"/AU
      OR "DEV D S"/AU OR "DEV D V"/AU) OR "DEV DEBAPRASAD"/AU
L5 ( 24) SEA FILE=HCAPLUS ABB=ON PLU=ON "MEDICHERIA SATYANARAYANA"/AU
      OR ("MEDICHERLA SATYA"/AU OR "MEDICHERLA SATYANANYANA"/AU OR
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L6 ( 433) SEA FILE=HCAPLUS ABB=ON PLU=ON (L1 OR L2 OR L3 OR L4 OR L5)
L7 ( 419) SEA FILE=HCAPLUS ABB=ON PLU=ON L6 AND (AY<2003 OR PY<2003 OR
      PRY<2003)
L8 ( 22) SEA FILE=HCAPLUS ABB=ON PLU=ON L7 AND ?DIABET?
L9 ( 11) SEA FILE=HCAPLUS ABB=ON PLU=ON L7 AND ?GLYCERID?
L10 11 SEA FILE=HCAPLUS ABB=ON PLU=ON L8 AND L9
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=> d que l22

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L11 ( 46) SEA FILE=BIOSIS ABB=ON PLU=ON ("NEOGI P"/AU OR "NEOGI P K
      B"/AU OR "NEOGI PARTHA"/AU)
L12 ( 131) SEA FILE=BIOSIS ABB=ON PLU=ON ("NAG B"/AU OR "NAG B L"/AU OR
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      "NAG BISWAJIT"/AU)
L13 ( 8) SEA FILE=BIOSIS ABB=ON PLU=ON ("LAKNER F J"/AU OR "LAKNER
      FRDERICK J"/AU OR "LAKNER FREDERICK J"/AU OR "LAKNER FREDRICK
      J"/AU)
L14 ( 44) SEA FILE=BIOSIS ABB=ON PLU=ON ("DEV D"/AU OR "DEV D G"/AU OR
      "DEV D K"/AU OR "DEV D S"/AU OR "DEV D V"/AU)
L15 ( 33) SEA FILE=BIOSIS ABB=ON PLU=ON "MEDICHERIA SATYA"/AU OR
      ("MEDICHERLA S"/AU OR "MEDICHERLA SATYA"/AU OR "MEDICHERLA
      SATYANANYANA"/AU OR "MEDICHERLA SATYANARAYANA"/AU)
L16 ( 220) SEA FILE=BIOSIS ABB=ON PLU=ON (L11 OR L12 OR L13 OR L14 OR
      L15)
L17 ( 11) SEA FILE=BIOSIS ABB=ON PLU=ON L16 AND ?GLYCERID?
L18 ( 148) SEA FILE=BIOSIS ABB=ON PLU=ON L16 AND (CONG? OR CONF? OR
      SYMP? OR MEET? OR MTG OR FORUM OR FORA OR ASSEM? OR WORK? OR
      WKSHP? OR COLLOQ? OR SESS? OR SEM? OR TRANS? OR PROC? OR ABS?
      OR REV?)/DT,SO,ST,CT,CW,IT,MT,BI
L19 ( 84) SEA FILE=BIOSIS ABB=ON PLU=ON L16 AND 00520/CC
L20 ( 85) SEA FILE=BIOSIS ABB=ON PLU=ON (L18 OR L19) NOT ARTICLE/DT
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L21 (7) SEA FILE=BIOSIS ABB=ON PLU=ON L20 AND ?GLYCER?
 L22 11 SEA FILE=BIOSIS ABB=ON PLU=ON L17 OR L21

=> dup rem l10 l22

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 PROCESSING COMPLETED FOR L10
 PROCESSING COMPLETED FOR L22

L23 20 DUP REM L10 L22 (2 DUPLICATES REMOVED)
 ANSWERS '1-11' FROM FILE HCAPLUS
 ANSWERS '12-20' FROM FILE BIOSIS

=> d ibib abs

L23 ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 1
 ACCESSION NUMBER: 2003:747894 HCAPLUS
 DOCUMENT NUMBER: 139:255379
 TITLE: Diphenylethylene compounds for the treatment of diabetes
 INVENTOR(S): Nag, Bishwajit; Medicherla,
 Satyanarayana; Dey, Debendranath
 PATENT ASSIGNEE(S): Calyx Therapeutics, Inc., USA
 SOURCE: U.S., 14 pp., Cont.-in-part of U.S. 6,245,814.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 9
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6624197	B1	20030923	US 2000-642618	20000817 <--
US 6245814	B1	20010612	US 1998-74925	19980508 <--
WO 2001056382	A1	20010809	WO 2001-US3797	20010205 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002002200	A1	20020103	US 2001-777551	20010205 <--
EP 1251738	A1	20021030	EP 2001-905454	20010205 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003521500	T2	20030715	JP 2001-556090	20010205 <--
PRIORITY APPLN. INFO.: US 1998-74925 A2 19980508 <-- US 2000-180340P P 20000204 <-- US 2000-642618 A 20000817 <-- WO 2001-US3797 W 20010205 <--				
OTHER SOURCE(S): MARPAT 139:255379				

AB Diphenylethylene and styrene compds. are provided which are administered orally to decrease blood glucose levels in rats. The glucose tolerance in insulin-resistant rats is also shown, as well as lowering of triglyceride levels in serum insulin-resistant, hyperinsulinemic and hypertriglyceridemic rats. The compds. are orally effective antidiabetic agents that potentially may reduce abnormality of glucose and lipid metabolism in diabetes. Preparation of 2-(4-hydroxyphenyl)-3-(3,5-dimethoxyphenyl)propenoic acid isomers and sodium salts is described.

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs 2-

YOU HAVE REQUESTED DATA FROM 19 ANSWERS - CONTINUE? Y/(N):y

L23 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2001:627250 HCAPLUS

DOCUMENT NUMBER: 135:162510

TITLE: Diphenylethylene and styrene compounds for the treatment of diabetes

INVENTOR(S): Nag, Bishwajit; Medicherla, Satyanarayana; Dey, Debendranath

PATENT ASSIGNEE(S): Calyx Therapeutics, Inc., USA

SOURCE: U.S., 9 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 9

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6245814	B1	20010612	US 1998-74925	19980508 <--
WO 9958127	A1	19991118	WO 1999-US9982	19990507 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9939741	A1	19991129	AU 1999-39741	19990507 <--
AU 751235	B2	20020808		
EP 1007039	A1	20000614	EP 1999-922836	19990507 <--
EP 1007039	B1	20040303		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002514598	T2	20020521	JP 2000-547978	19990507 <--
AT 260906	E	20040315	AT 1999-922836	19990507 <--
NZ 511065	A	20030829	NZ 1999-511065	19990518 <--
US 6624197	B1	20030923	US 2000-642618	20000817 <--
US 2002025975	A1	20020228	US 2001-785554	20010220 <--
US 2002032225	A1	20020314	US 2001-843167	20010427 <--
PRIORITY APPLN. INFO.:			US 1998-74925 A 19980508 <--	
			US 1999-287237 A 19990406 <--	
			WO 1999-US9982 W 19990507 <--	
			US 2000-591105 A2 20000609 <--	
			US 2001-785554 A2 20010220 <--	

OTHER SOURCE(S) : MARPAT 135:162510

AB Novel diphenylethylene and styrenes are provided which are administered orally to decrease blood glucose levels in rats. The glucose tolerance in insulin resistant rats is also shown, as well as lowering of **triglyceride** levels in serum insulin resistant, hyperinsulinemic and hypertriglyceridemic rats. The compds. are orally effective anti-**diabetic** agents that potentially may reduce abnormality of glucose and lipid metabolism in **diabetes**.

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 3 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:757334 HCPLUS

DOCUMENT NUMBER: 139:276885

TITLE: Preparation of novel heterocyclic analogs of diphenylethylene compounds as **antidiabetics**

INVENTOR(S) : Neogi, Partha; Dey, Debendranath; Medicherla, Satyanarayana; Nag, Bishwajit; Lee, Arthur

PATENT ASSIGNEE(S) : USA

SOURCE: U.S. Pat. Appl. Publ., 66 pp., Cont.-in-part of U.S. Ser. No. 843,167.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 9

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003181494	A1	20030925	US 2002-265902	20021008 <--
US 2002025975	A1	20020228	US 2001-785554	20010220 <--
US 2002032225	A1	20020314	US 2001-843167	20010427 <--
WO 2004033438	A1	20040422	WO 2003-US31803	20031008 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO. :			US 1999-287237	A2 19990406 <--
			US 2000-591105	B2 20000609 <--
			US 2001-785554	A2 20010220 <--
			US 2001-843167	A2 20010427 <--
			US 1998-74925	A2 19980508 <--
			US 2002-265902	A2 20021008 <--

OTHER SOURCE(S) : MARPAT 139:276885

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; Z = II-IV; n, m, q and r = 0-4 (n+m ≤ 4 and

$q+r \leq 4$; $p, s = 0-5$ ($p+s \leq 5$); $R, R2 = H, alkyl, alkenyl, etc.$; $R1 = H, alkyl, alkenyl, etc.$; $A, A1, A2 = H, acylamino, acyloxy, alkanoyl, etc.$; $B, B1, B2 = H, acylamino, acyloxy, alkanoyl, etc.$; or A and B together, or $A1$ and $B1$ together, or $A2$ and $B2$ together, may be joined to form a methylenedioxy or ethylenedioxy; $X, X1 = (un)substituted NH, O, S$ which are effective in lowering blood glucose level, serum insulin, triglyceride and free fatty acid levels in animal models of Type II diabetes, were prepared E.g., a multi-step synthesis of V, starting from 3,5-dimethoxybenzaldehyde and 4-hydroxyphenylacetic acid, was given. The compound V showed strong glucose lowering activity even though it is a weak PPAR- γ agonist (data given). The compds. I are disclosed as useful for a variety of treatments including the treatment of inflammation, inflammatory and immunol. diseases, insulin resistance, hyperlipidemia, coronary artery disease, cancer and multiple sclerosis. Pharmaceutical composition comprising the compound I was claimed.

L23 ANSWER 4 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:185699 HCPLUS

DOCUMENT NUMBER: 136:247571

TITLE: Preparation of novel heterocyclic analogs of diphenylethylene compounds as inhibitors of cytokines or cyclooxygenase

INVENTOR(S): Nag, Bishwajit; Dey, Debendranath;
Medicherla, Satyanarayana; Neogi,
Partha

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 34 pp., Cont.-in-part of U.S.
Ser. No. 785,554.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 9

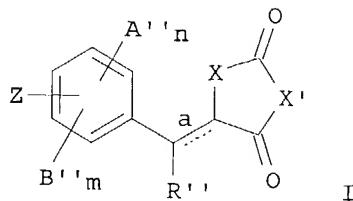
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 6245814	B1	20010612	US 1998-74925	19980508 <--
US 2002025975	A1	20020228	US 2001-785554	20010220 <--
WO 2001095859	A2	20011220	WO 2001-US17950	20010605 <--
WO 2001095859	A3	20030828		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2001066670	A5	20011224	AU 2001-66670	20010605 <--
EP 1360178	A2	20031112	EP 2001-944241	20010605 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
US 2003181494	A1	20030925	US 2002-265902	20021008 <--
PRIORITY APPLN. INFO.:			US 1998-74925	A2 19980508 <--
			US 1999-287237	A2 19990406 <--
			US 2000-591105	A2 20000609 <--
			US 2001-785554	A2 20010220 <--

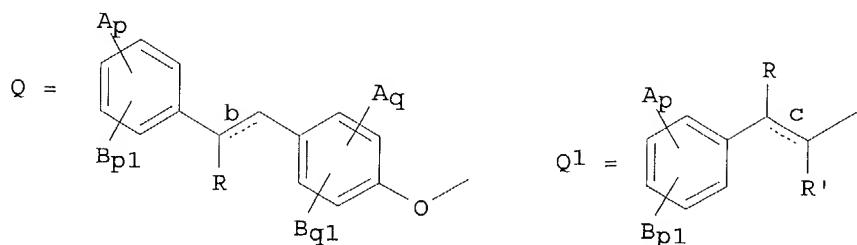
US 2001-843167 A2 20010427 <--
 WO 2001-US17950 W 20010605 <--

OTHER SOURCE(S) :
 GI

MARPAT 136:247571



W



AB Novel diphenylethylene compds. and derivs. thereof containing thiazolidinedione or oxazolidinedione moieties are provided which are effective in lowering blood glucose level, serum insulin, triglyceride and free fatty acid levels in animal models of Type II diabetes. The above compds. and their derivs. are represented by formula [I; Z = Q, Q1, H, A'', B''; wherein n, m, q, q1 = integers from zero to 4 provided that $n+m \leq 4$ and $q+q1 \leq 4$; p, p1 = integers from zero to 5 provided that $p+p1 \leq 5$; a, b and c are double bonds which may be present or absent; when present; the double bonds may be in the E or Z configuration and, when absent, the resulting stereocenters may have the R- or S- configuration; R, R', R'' = H, C1-20 linear or branched alkyl, C2-20 linear or branched alkenyl, CO2Z' (wherein Z' = H, Na, K, or other pharmaceutically acceptable counterion such as Ca, Mg, ammonium, tromethamine, and the like), CO2R''', NH2, NHR''', N(R''')2, OH, OR''', halo, substituted C1-20 linear or branched alkyl or substituted C2-20 linear or branched alkenyl (wherein R''' is C1-20 linear or branched alkyl or linear or branched alkenyl); A, A', A'' = H, C1-20 acylamino, C1-20 acyloxy, C1-20 alkanoyl, C1-20 alkoxy carbonyl, C1-20 alkoxy, C1-20 alkylamino, C1-20 alkylcarboxylamino, CO2H, cyano, halo, HO; B, B', B'' = H, C1-20 acylamino, C1-20 acyloxy, C1-20 alkanoyl, C1-20 alkenoyl, C1-20 alkoxy carbonyl, C1-20 alkoxy, C1-20 alkylamino, C1-20 alkylcarboxylamino, aroyl, aralkanoyl, CO2H, cyano, halo, HO; or A and B together, or A' and B' together, or A'' and B'' together, may be joined to form a methylenedioxy or ethylenedioxy group; and X, X' are independently -NH, -NR''', O or S]. In contrast to previously reported thiazolidinedione compds., known to lower leptin levels, the present compds. increase leptin levels and have no known liver toxicity. They inhibit the activity of TNF-alpha, interleukin IL-1 or IL-6 or cyclooxygenase-2 (COX-2). The compds. are disclosed as useful for a variety of treatments including the treatment of inflammation, inflammatory and immunol. diseases, insulin resistance, hyperlipidemia, coronary artery disease, cancer and multiple sclerosis. Thus, To a mixture of 3,5-dimethoxybenzaldehyde (500 g) and

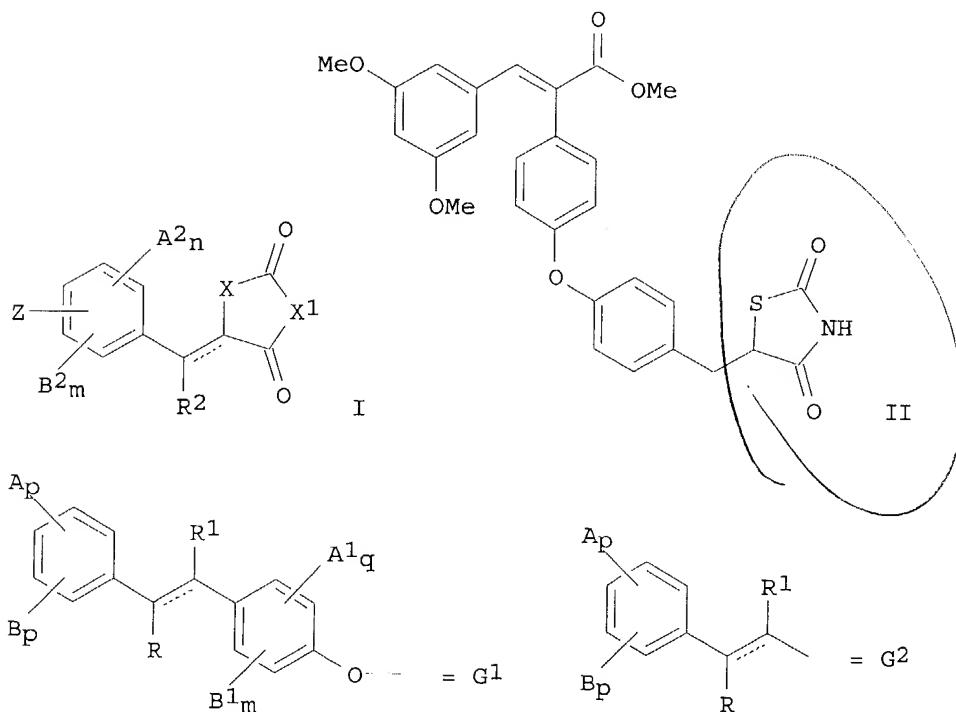
p-hydroxyphenylacetic acid (457 g) was added acetic anhydride (1 L) and triethylamine (420 mL) and the nonhomogeneous mixture on heating became homogeneous at 70° and stirred at 130-140° for 6 h to give 47% 3-(3,5-dimethoxyphenyl)-2-(4-hydroxyphenyl)acrylic acid (II) (428 g). II (427.5 g) was suspended in 3 L methanol, treated with 100 mL concentrated H₂SO₄, and heated at reflux for 20 h under Ar to give 97% 3-(3,5-dimethoxyphenyl)-2-(4-hydroxyphenyl)acrylic acid Me ester (III). III (433 g) was dissolved in 1.6 L DMF, treated with 60.4 g NaH (50% in oil) and the with 185 mL p-fluorobenzaldehyde, and heated at 180° for 18 h to give 77% 3-(3,5-dimethoxyphenyl)-2-[4-(4-formylphenoxy)phenyl]acrylic acid Me ester which (352 g), 2,4-thiazolidinedione 98.6, benzoic acid 134, and piperidine 107.4 g were heated in 2.5 L toluene at reflux with continuous removal of H₂O through Dean-Stark apparatus to give 86% 3-(3,5-dimethoxyphenyl)-2-[4-[4-(2,4-dioxothiazolidin-5-ylidenemethyl)phenoxy]phenyl]acrylic acid Me ester (IV). IV (30 g) was hydrogenated over 15 g 10% Pd-C in 900 mL dioxane in a Parr apparatus at 60 Psi for 24 h, followed by adding 15 g 10% Pd-C and continuing the hydrogenation for another 24 h to give 86% 3-(3,5-dimethoxyphenyl)-2-[4-[4-(2,4-dioxothiazolidin-5-ylmethyl)phenoxy]phenyl]acrylic acid Me ester (V). When V was orally administered to ob/ob mice with a single oral dose (50 mg/kg body weight), there was a 62 % drop in blood glucose level and, similar to db/db mice, there was no significant increase in body weight between the control and the treatment groups. This was in contrast to treatment of **diabetic** animals by thiazolidinedione type compds. which are known to be associated with increase in body weight

L23 ANSWER 5 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2002:158391 HCAPLUS
 DOCUMENT NUMBER: 136:216745
 TITLE: Preparation and activity of diphenylethylene thiazolidinediones and analogs as antidiabetics, antiinflammatories, or immunomodulators
 INVENTOR(S): Nag, Bishwajit; Dey, Debendranath;
 Medicherla, Satyanarayana; Neogi, Partha
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 30 pp., Cont.-in-part of U.S.
 Ser. No. 591,105.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 9
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002025975	A1	20020228	US 2001-785554	20010220 <--
US 6245814	B1	20010612	US 1998-74925	19980508 <--
US 2002032225	A1	20020314	US 2001-843167	20010427 <--
WO 2001095859	A2	20011220	WO 2001-US17950	20010605 <--
WO 2001095859	A3	20030828		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,			

DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
 AU 2001066670 A5 20011224 AU 2001-66670 20010605 <--
 EP 1360178 A2 20031112 EP 2001-944241 20010605 <--
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, FI, CY, TR
 US 2003181494 A1 20030925 US 2002-265902 20021008 <--
 PRIORITY APPLN. INFO.: US 1998-74925 A2 19980508 <--
 US 1999-287237 A2 19990406 <--
 US 2000-591105 A2 20000609 <--
 US 2001-785554 A2 20010220 <--
 US 2001-843167 A2 20010427 <--
 WO 2001-US17950 W 20010605 <--

OTHER SOURCE(S) : MARPAT 136:216745
 GI

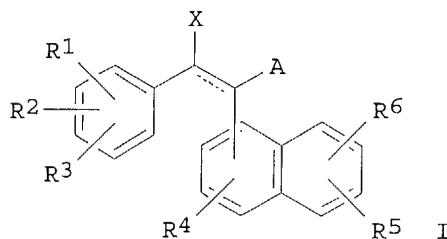


AB Title compds. I [wherein Z = G1, H, A2, B2, or G2; n, m, and q = independently 0-4; p = independently 0-5; R, R1, and R2 = independently H, (un)substituted alkyl or alkenyl, CO₂Z1, CO₂R3, NH₂, NHR3, NR₃2, OH, OR₃, or halo; Z1 = H, Na, K, or other pharmaceutically acceptable counterion; R3 = alkyl or alkenyl; A, A1, and A2 = independently H, acylamino, acyloxy, alkanoyl, alkoxy carbonyl, alkoxy, alkylamino, alkylcarboxylamino, carboxyl, CN, H, or OH; B, B1, and B2 = independently H, acylamino, acyloxy, alkanoyl, alkenoyl, alkoxy carbonyl, alkoxy, alkylamino, alkylcarboxylamino, aroyl, aralkanoyl, carboxyl, CN, halo, or OH; or A and B or A1 and B1 or A2 and B2 together form a methylenedioxy or ethylenedioxy group; X and X1 = independently NH, NR₃, O, or S] are provided which are effective in lowering blood glucose level, serum

insulin, triglyceride, and free fatty acid levels in animal models of Type II diabetes. In contrast to previously reported thiazolidinedione compds., known to lower leptin levels, the present compds. increase leptin levels and have no known liver toxicity. Thus, II was prepared in five steps by condensation of 3,5-dimethoxybenzaldehyde with 4-hydroxyphenylacetic acid (47%), followed by esterification (97%), etherification with 4-fluorobenzaldehyde (77%), condensation with 2,4-thiazolidinedione (86%), and hydrogenation of the ylidene double bond (40%). Oral administration of II to obese mice caused a 62% drop in blood glucose level. I are useful for the treatment of inflammation, inflammatory and immunol. diseases, insulin resistance, hyperlipidemia, coronary artery disease, cancer, and multiple sclerosis.

L23 ANSWER 6 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2002:11108 HCPLUS
 DOCUMENT NUMBER: 136:69654
 TITLE: Preparation of diphenylethylene compounds as antidiabetic agents
 INVENTOR(S): Nag, Bishwagit; Dey, Debendranath;
 Medicherla, Satyanarayana; Neogi, Partha
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 38 pp., Cont.-in-part of U.S.
 Ser. No. 642,618.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 9
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002002200	A1	20020103	US 2001-777551	20010205 <--
US 6624197	B1	20030923	US 2000-642618	20000817 <--
PRIORITY APPLN. INFO.:			US 2000-180340P	P 20000204 <--
			US 2000-642618	A2 20000817 <--
			US 1998-74925	A2 19980508 <--
OTHER SOURCE(S):		MARPAT 136:69654		
GI				



AB Title compds. I [wherein A = CO₂R, CONR'R'', CN, or COR₂; X = H, OH, or (un)substituted alkyl or alkenyl; R = H, (ar)alkyl, or aryl; R₁, R₂, R₃, R₄, R₅, R₆, and R₇ = independently H, (un)substituted alkyl or alkenyl; CO₂R, NR'R'', or CONCR'R''; R' and R'' = independently H, alkyl, aryl, OH, alkoxy, acylamino, acyloxy, alkanoyl, alkoxy carbonyl, halo, NO₂, SO₂R'''; CZ₃; Z = independently H, halo, (halo)alkyl, or SR'''; R''' = H or alkyl; or R₂ and R₃ together or R₅ and R₆ together may be joined to form

(m) ethylenedioxy; with provisos; and E and Z isomers thereof] were prepared and shown to decrease circulating concns. of glucose when administered orally. For instance, 3,5-dimethoxybenzaldehyde was coupled with p-hydroxyphenyl acetic acid using TEA in acetic anhydride to give (E)-3-(3,5-dimethoxyphenyl)-2-(4-hydroxyphenyl)acrylic acid (II), which exhibited glucose-lowering effects for more than 15 days at a dose of 20 mg/kg p.o. Examples also include twenty-six bioassays, such as studies on the effects of II on insulin resistant rats, lipid and leptin concns., PPAR binding, overexpression of the human insulin-like growth factor 1 receptor and human insulin receptor, toxicity, and kinetics of drug absorption. I are orally effective antidiabetic agents that normalize glucose and lipid metabolism

L23 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:923567 HCAPLUS

DOCUMENT NUMBER: 136:37596

TITLE: Preparation and activity of diphenylethylene thiazolidinedione or oxazolidinedione compounds as antidiabetics or antiinflammatories

INVENTOR(S): Neogi, Partha; Nag, Bishwajit;

Medicherla, Satyanarayana; Dey, Debendranath Calyx Therapeutics, Inc., USA

SOURCE: PCT Int. Appl., 76 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

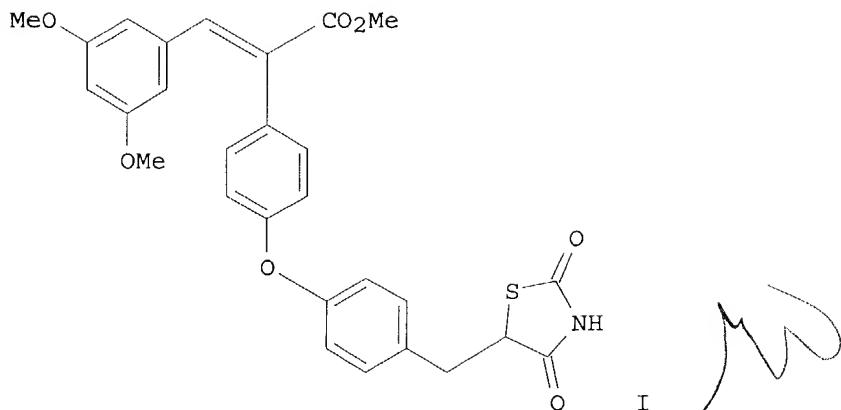
FAMILY ACC. NUM. COUNT: 9

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001095859	A2	20011220	WO 2001-US17950	20010605 <--
WO 2001095859	A3	20030828		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002025975	A1	20020228	US 2001-785554	20010220 <--
US 2002032225	A1	20020314	US 2001-843167	20010427 <--
AU 2001066670	A5	20011224	AU 2001-66670	20010605 <--
EP 1360178	A2	20031112	EP 2001-944241	20010605 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
PRIORITY APPLN. INFO.:			US 2000-591105	A2 20000609 <--
			US 2001-785554	A2 20010220 <--
			US 2001-843167	A2 20010427 <--
			US 1998-74925	A2 19980508 <--
			US 1999-287237	A2 19990406 <--
			WO 2001-US17950	W 20010605 <--

OTHER SOURCE(S): MARPAT 136:37596

GI



AB Novel diphenylethylene compds. and derivs. thereof containing thiazolidinedione or oxazolidinedione moieties are provided which are effective in lowering blood glucose level, serum insulin, **triglyceride** and free fatty acid levels in animal models of Type II diabetes. In contrast to previously reported thiazolidinedione compds., known to lower leptin levels, the present compds. increase leptin levels and have no known liver toxicity. Thus, (I) was prepared in five steps by condensation of 3,5-dimethoxybenzaldehyde with 4-hydroxyphenylacetic acid followed by esterification and etherification with 4-fluorobenzaldehyde and condensation with 2,4-thiazolidinedione and hydrogenation of the ylidene double bond. Oral administration of I to obese mice caused a 62% drop in blood glucose level. The compds. are disclosed as useful for a variety of treatments including the treatment of inflammation, inflammatory and immunol. diseases, insulin resistance, hyperlipidemia, coronary artery disease, cancer and multiple sclerosis.

L23 ANSWER 8 OF 20 HCAPLUS COPYRIGHT 2004 ACS ON STN

ACCESSION NUMBER: 2001:581654 HCAPLUS
 DOCUMENT NUMBER: 135:147444
 TITLE: Novel diphenylethylene compounds
 INVENTOR(S): Nag, Bishwajit; Dey, Debendranath;
 Medicherla, Satyanarayana
 PATENT ASSIGNEE(S): Calyx Therapeutics, Inc., USA
 SOURCE: PCT Int. Appl., 55 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 9
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001056382	A1	20010809	WO 2001-US3797	20010205 <--
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,			

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 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
 US 6624197 B1 20030923 US 2000-642618 20000817 <--
 EP 1251738 A1 20021030 EP 2001-905454 20010205 <--
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 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
 JP 2003521500 T2 20030715 JP 2001-556090 20010205 <--
 PRIORITY APPLN. INFO.: US 2000-180340P P 20000204 <--
 US 2000-642618 A 20000817 <--
 US 1998-74925 A2 19980508 <--
 WO 2001-US3797 W 20010205 <--

OTHER SOURCE(S) : MARPAT 135:147444

AB Novel diphenylethylene compds. that are administered orally to decrease circulating concns. of glucose are provided. The effect on insulin resistant rats is also shown. The effects on lipid and leptin concns. are also shown. The compds. are orally effective anti-diabetic agents that may normalize glucose and lipid metabolism in subjects with diabetes.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 9 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:359750 HCPLUS

DOCUMENT NUMBER: 134:348284

TITLE: Phenyl compounds to treat diabetes and associated conditions

INVENTOR(S) : Neogi, Partha; Nag, Bishwajit;
 Lakner, Frederick J.; Dey, Debendranath;
 Medicherla, Satyanarayana

PATENT ASSIGNEE(S) : Calyx Therapeutics, Inc., USA

SOURCE: PCT Int. Appl., 47 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

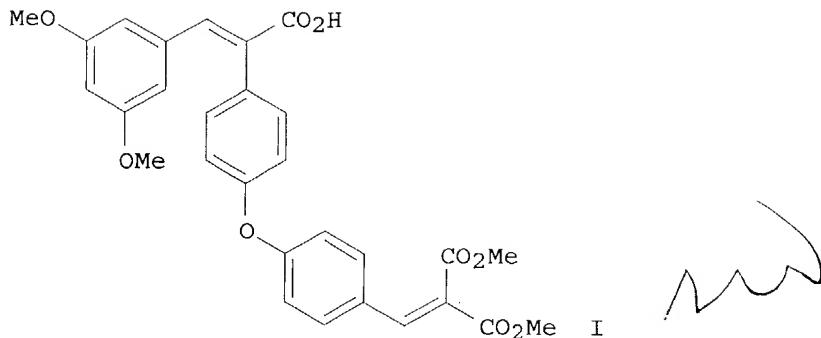
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2001034094	A2	20010517	WO 2000-US30927	20001108 <--
WO 2001034094	C2	20020725		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6525093	B1	20030225	US 1999-436047	19991108 <--
AU 2001017607	A5	20010606	AU 2001-17607	20001108 <--
EP 1235785	A2	20020904	EP 2000-980331	20001108 <--
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JP 2004503464	T2	20040205	JP 2001-536099	20001108 <--
US 2002107285	A1	20020808	US 2002-75442	20020215 <--
PRIORITY APPLN. INFO.:			US 1999-436047	A 19991108 <--
OTHER SOURCE(S) :	MARPAT 134:348284		WO 2000-US30927	W 20001108 <--

GI



AB Ph compds. (Markush included) are provided that lower blood glucose concns., lower serum **triglyceride** concns., lower systolic blood pressure, and increase glucose uptake by adipose tissue, but do not affect the expression of PPAR- γ by adipose tissue. Compds. of the invention include e.g. I.

L23 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:824099 HCAPLUS

DOCUMENT NUMBER: 133:362623

TITLE: Diphenylethylenes and styrenes for decreasing blood glucose levels

INVENTOR(S): Nag, Bishwajit; Medicherla,

Satyana Rayana; Dey, Debendranath

PATENT ASSIGNEE(S): Calyx Therapeutics, Inc., USA

SOURCE: PCT Int. Appl., 27 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

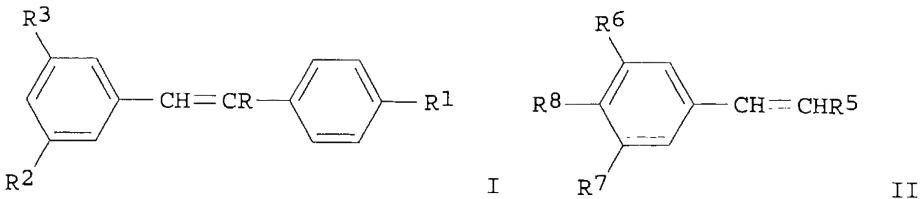
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000069430	A1	20001123	WO 1999-US11001	19990518 <--
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AU 9940857	A1	20001205	AU 1999-40857	19990518 <--
EP 1178788	A1	20020213	EP 1999-924332	19990518 <--
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JP 2002544227	T2	20021224	JP 2000-617889	19990518 <--
PRIORITY APPLN. INFO.:			WO 1999-US11001	A 19990518 <--
OTHER SOURCE(S):		MARPAT 133:362623		

GI



AB Diphenylethylenes I ($R = H, CO_2H, CO_2Na$, etc.; $R1, R2, R3 = H, OH, alkoxy$; when $R = H$ and $R2 = R3 = MeO$, $R1$ is not OH) and styrenes II ($R5 = H, Me$; $R6, R7 = H, MeO$; $R8 = H, OH$) were prepared as **antidiabetic** agents. Thus, reaction of 3,5-dimethoxybenzaldehyde with (4-hydroxyphenyl)acetic acid in $AcOH-Et_3N$ at $130-140^\circ$ for 24 h gave I ($R = CO_2H, R1 = OH, R2 = R3 = MeO$), which was decarboxylated by refluxing with Cu in quinoline and was converted to the Na salt by reaction with NaOH at room temperature. The styrenes were prepared by Wittig reactions of benzaldehydes. I ($R = CO_2Na, R1 = OH, R2 = R3 = MeO$) reduced blood glucose, plasma **triglyceride**, and plasma insulin levels in rats and improved glucose tolerance in insulin-resistant obese rats.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 11 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:736478 HCPLUS

DOCUMENT NUMBER: 131:332116

TITLE: Heterocyclic analogs of diphenylethylene compounds for the treatment of **diabetes**

INVENTOR(S): Neogi, Partha; Nag, Bishwajit;

PATENT ASSIGNEE(S): Medicherla, Satyanarayana; Dey, Debendranath
Calyx Therapeutics, Inc., USA

SOURCE: PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 9

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9958127	A1	19991118	WO 1999-US9982	19990507 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6245814	B1	20010612	US 1998-74925	19980508 <--
AU 9939741	A1	19991129	AU 1999-39741	19990507 <--
AU 751235	B2	20020808		
EP 1007039	A1	20000614	EP 1999-922836	19990507 <--
EP 1007039	B1	20040303		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				

JP 2002514598	T2	20020521	JP 2000-547978	19990507 <--
AT 260906	E	20040315	AT 1999-922836	19990507 <--
PRIORITY APPLN. INFO.:			US 1998-74925	A 19980508 <--
			US 1999-287237	A 19990406 <--
			WO 1999-US9982	W 19990507 <--

OTHER SOURCE(S) : MARPAT 131:332116

AB Diphenylethylene compds. containing thiazolidinedione or oxazolidinedione moieties are provided which are effective in lowering blood glucose level, serum insulin, **triglyceride** and free fatty acid levels in animal models of Type II **diabetes**. In contrast to previously reported thiazolidine compds., known to lower leptin levels, the present compds. increase leptin levels and have no known liver toxicity.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 12 OF 20 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
ACCESSION NUMBER: 2003:162019 BIOSIS

DOCUMENT NUMBER: PREV200300162019

TITLE: Compounds to treat diabetes and associated conditions.

AUTHOR(S) : Neogi, Partha [Inventor, Reprint Author];
Nag, Bishwajit [Inventor]; Lakner, Frederick
J. [Inventor]; Dey, Debendranath [Inventor];
Medicherla, Satyanarayana [Inventor]

CORPORATE SOURCE: Hayward, CA, USA

ASSIGNEE: Calyx Therapeutics Inc.

PATENT INFORMATION: US 6525093 February 25, 2003

SOURCE: Official Gazette of the United States Patent and Trademark Office Patents, (Feb 25 2003) Vol. 1267, No. 4.
<http://www.uspto.gov/web/menu/patdata.html>. e-file.

ISSN: 0098-1133 (ISSN print).

DOCUMENT TYPE: Patent

LANGUAGE: English

ENTRY DATE: Entered STN: 26 Mar 2003

Last Updated on STN: 26 Mar 2003

AB Compounds are provided that lower blood glucose concentrations, lower serum **triglyceride** concentrations, lower systolic blood pressure, and increase glucose uptake by adipose tissue, but do not affect the expression of PPAR-gamma by adipose tissue.

L23 ANSWER 13 OF 20 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
ACCESSION NUMBER: 2003:459396 BIOSIS

DOCUMENT NUMBER: PREV200300459396

TITLE: BLX-1002: A new class of orally-active anti-diabetic small molecule with no PPAR-gamma affinity.

AUTHOR(S) : Pandey, Bindu [Reprint Author]; Nag, Abhijeet [Reprint Author]; Singh, Ashmika [Reprint Author]; Vargas, Hyang [Reprint Author]; Gutala, Sreekanth [Reprint Author]; Dey, Deben [Reprint Author]; Nag, Bishwajit [Reprint Author]

CORPORATE SOURCE: Union City, CA, USA

SOURCE: Diabetes, (2003) Vol. 52, No. Supplement 1, pp. A143.
print.

Meeting Info.: 63rd Scientific Sessions of the American Diabetes Association. New Orleans, LA, USA.
June 13-17, 2003. American Diabetes Association.

ISSN: 0012-1797 (ISSN print).

DOCUMENT TYPE: Conference; (Meeting)

Conference; (Meeting Poster)

Conference; Abstract; (Meeting Abstract)

LANGUAGE: English

ENTRY DATE: Entered STN: 8 Oct 2003
 Last Updated on STN: 8 Oct 2003

L23 ANSWER 14 OF 20 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
 ACCESSION NUMBER: 2003:531294 BIOSIS
 DOCUMENT NUMBER: PREV200300531302
 TITLE: A nonadipogenic compound BLX-1002 induces glucose uptake in 3T3-L1 cells and has strong anti-hyperglycemic effect in db/db and ob/ob mice.
 AUTHOR(S): Dey, D. [Reprint Author]; Gupta, A.; Pandey, B.; Nag, A. [Reprint Author]; Agarwal, S. K.; Nag, B. [Reprint Author]
 CORPORATE SOURCE: Research and Development, Bexel Pharmaceuticals Inc., Union City, CA, USA
 SOURCE: Diabetologia, (August 2003) Vol. 46, No. Supplement 2, pp. A 300. print.
 Meeting Info.: 18th Congress of the International Diabetes Federation. Paris, France. August 24-29, 2003. International Diabetes Federation.
 CODEN: DBTGAI. ISSN: 0012-186X.

DOCUMENT TYPE: Conference; (Meeting)
 Conference; Abstract; (Meeting Abstract)

LANGUAGE: English
 ENTRY DATE: Entered STN: 12 Nov 2003
 Last Updated on STN: 12 Nov 2003

L23 ANSWER 15 OF 20 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
 ACCESSION NUMBER: 2002:370349 BIOSIS
 DOCUMENT NUMBER: PREV200200370349
 TITLE: SleemaX: A new herbamin formulation as an anti-obese alternative medicine with hypolipidemic and insulin sensitizing properties.
 AUTHOR(S): Nag, Abhijeet [Reprint author]; Nag, Nitish [Reprint author]; Nag, Bishwajit [Reprint author]
 CORPORATE SOURCE: BEXEL Biotechnology, Inc., 29552 Union City Blvd., Union City, CA, 94587, USA
 SOURCE: FASEB Journal, (March 22, 2002) Vol. 16, No. 5, pp. A1017. print.
 Meeting Info.: Annual Meeting of Professional Research Scientists on Experimental Biology. New Orleans, Louisiana, USA. April 20-24, 2002.
 CODEN: FAJOEC. ISSN: 0892-6638.

DOCUMENT TYPE: Conference; (Meeting)
 Conference; Abstract; (Meeting Abstract)

LANGUAGE: English
 ENTRY DATE: Entered STN: 3 Jul 2002
 Last Updated on STN: 3 Jul 2002

AB Obesity is a chronic disorder characterized by several parameters such as overabundance of adipose tissue, high triglycerides, and link with insulin resistance. Obesity is linked with hypertension, coronary heart disease and diabetes. Limited medications are available to tackle this huge growing concern in developed countries. Studies show that a number of herbs and minerals may play a key role in lowering body fat mass in obese people. SleemaX was formulated with two natural product extracts in combination with mineral ions and unusual amino acids. When given orally to ob/ob mice for a period of three weeks, SleemaX lowered body weight by 10% without any change in daily food and water intake. SleemaX reduced hyperinsulinemia by 52%, total cholesterol by 28%, serum triglycerides by 42% and basal blood glucose concentration by 44% in ob/ob mice. In a fasting stage, ob/ob mice treated with SleemaX for 2

weeks showed a significant improvement in oral glucose tolerance at all time points. These results indicate that daily oral administration of SleemaX can lower body weight and ameliorate the insulin resistance in mature onset of obesity. The mechanism of SleemaX action is currently being investigated. With no change in food uptake in these animals, SleemaX has the potential as a non-appetite suppressive alternative medicine for the management of obesity.

L23 ANSWER 16 OF 20 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
 ACCESSION NUMBER: 2002:396559 BIOSIS
 DOCUMENT NUMBER: PREV200200396559
 TITLE: Dichol improves glucose homeostasis, insulin sensitivity, and restores lipid balance in two genetic rodent models of type II diabetes.
 AUTHOR(S): Nag, Bishwajit [Reprint author]; Medicherla, Satya [Reprint author]; Nag, Abhijeet [Reprint author]
 CORPORATE SOURCE: BEXEL Biotechnology, Inc., 29552 Union City Blvd., Union City, CA, 94587, USA
 SOURCE: FASEB Journal, (March 20, 2002) Vol. 16, No. 4, pp. A647-A648. print.
 Meeting Info.: Annual Meeting of the Professional Research Scientists on Experimental Biology. New Orleans, Louisiana, USA. April 20-24, 2002.
 CODEN: FAJOEC. ISSN: 0892-6638.
 DOCUMENT TYPE: Conference; (Meeting)
 Conference; Abstract; (Meeting Abstract)
 LANGUAGE: English
 ENTRY DATE: Entered STN: 24 Jul 2002
 Last Updated on STN: 24 Jul 2002
 AB Type II diabetes is a complex metabolic disorder involving hyperglycemia with progressive development of insulin resistance, and is linked with a cascade of other metabolic defects leading to hypertension and hyperlipidemia. Dichol is a herbamin formulation containing two natural product extracts in combination with trace metal ions and relevant amino acids. The efficacy of Dichol was examined in diabetic db/db and ob/ob mice. Single dose oral administration of Dichol for 2 weeks at a dose of 500 mg/kg resulted in >40% and >30% transient correction of hyperglycemia in db/db and ob/ob mice. Unlike many antidiabetic drugs where body weight gain occurs, formulated Dichol treatment was attributed with reduction in body weight gain in both ob/ob and db/db mice models. Oral administration of Dichol in db/db and ob/ob mice resulted in improvement in glucose tolerance, lowering of triglycerides (50-61%) and total cholesterol (20-52%). In addition, Dichol treatment increased HDL concentrations in db/db mice (32%) but not in ob/ob mice. Long term treatment (15-21 days) with therapeutic dose reduced food intake in both db/db and ob/ob mice. Although the mechanism of Dichol action is not yet defined, results demonstrate the feasibility of discovering a novel insulin sensitizing herbamin that may lead to new alternative therapies for diabetes associated with hyperlipidemia.

L23 ANSWER 17 OF 20 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
 ACCESSION NUMBER: 2002:134506 BIOSIS
 DOCUMENT NUMBER: PREV200200134506
 TITLE: Heterocyclic analogs of diphenylethylene compounds.
 AUTHOR(S): Neogi, Partha [Inventor, Reprint author]; Nag, Bishwajit [Inventor]; Medicherla, Satyanarayana [Inventor]; Dey, Debendranath [Inventor]
 CORPORATE SOURCE: Fremont, CA, USA
 ASSIGNEE: Calyx Therapeutics Inc., Hayward, CA, USA
 PATENT INFORMATION: US 6331633 December 18, 2001

SOURCE: Official Gazette of the United States Patent and Trademark Office Patents, (Dec. 18, 2001) Vol. 1253, No. 3.
<http://www.uspto.gov/web/menu/patdata.html>. e-file.
CODEN: OGUPE7. ISSN: 0098-1133.

DOCUMENT TYPE: Patent

LANGUAGE: English

ENTRY DATE: Entered STN: 6 Feb 2002

Last Updated on STN: 26 Feb 2002

AB Novel diphenylethylene compounds containing thiazolidinedione or oxazolidinedione moieties are provided which are effective in lowering blood glucose level, serum insulin, triglyceride and free fatty acid levels in animal models of Type II diabetes. In contrast to previously reported thiazolidine compounds, known to lower leptin levels, the present compound increase leptin levels and have no known liver toxicity.

L23 ANSWER 18 OF 20 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
ACCESSION NUMBER: 2001:297270 BIOSIS

DOCUMENT NUMBER: PREV200100297270

TITLE: Evidence for the interaction of a small molecule with insulin receptor using surface plasmon resonance.

AUTHOR(S): Dey, Deben [Reprint author]; Neogi, Partha [Reprint author]; Nag, Bishwajit [Reprint author]

CORPORATE SOURCE: Calyx Therapeutics Inc., 3525 Breakwater Avenue, Hayward, CA, 94545, USA

SOURCE: FASEB Journal, (March 7, 2001) Vol. 15, No. 4, pp. A526. print.

Meeting Info.: Annual Meeting of the Federation of American Societies for Experimental Biology on Experimental Biology 2001. Orlando, Florida, USA. March 31-April 04, 2001.

CODEN: FAJOEC. ISSN: 0892-6638.

DOCUMENT TYPE: Conference; (Meeting)
Conference; Abstract; (Meeting Abstract)

LANGUAGE: English

ENTRY DATE: Entered STN: 20 Jun 2001

Last Updated on STN: 19 Feb 2002

AB CLX-0901, a synthetic water-soluble analog of a compound (CLX-0900) isolated from the heartwood of a plant, has been shown to lower blood glucose, triglyceride and free fatty acid concentrations in several animal models of type II diabetes. In addition, we have previously shown that CLX-0901, like insulin, stimulated rapid glucose uptake (within 30 minutes) in primary rat adipocytes and this uptake is inhibited by known PI 3-kinase inhibitors. CLX-0901, in a manner similar to insulin, also stimulated Akt activation and GLUT-4 translocation in 3T3-L1 adipocytes. To demonstrate whether these findings are due to direct interaction of CLX-0901 with the insulin receptor (IR), a cell-free system that utilizes surface plasmon resonance measurements was employed. The IR and the insulin-like growth factor binding protein-1 (IGFBP-1), used as a control surface, were immobilized by amine coupling to the dextran matrix of a CM5 sensor chip, and the remaining active groups were blocked with 1 M ethanolamine (pH 8.5). Varying concentrations of either insulin or CLX-0901 in PBS were injected at a flow rate of 20 micro liter/min for 2 minutes over the immobilized surfaces. Dose response curves of insulin and CLX-0901 were very similar, but the affinity of CLX-0901 for IR was 1000-fold less than that of insulin. Addition of CLX-0901 to the IGFBP-1 surface did not induce a response. To further confirm the specificity of these interactions, insulin-like growth factor-1 (IGF-1) was also injected over both surfaces. Passage of IGF-1 over an IGFBP-1 surface induced a

response to IGFBP-1 but not to IR. Several additional compounds known not to interact with IR, such as tolbutamide and an eighteen-amino-acid peptide with insulin-like activity (CLX-0100), showed no interaction with any of the surfaces. These results provide evidence that CLX-0901 selectively binds to the insulin receptor.

L23 ANSWER 19 OF 20 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
 ACCESSION NUMBER: 2001:449945 BIOSIS
 DOCUMENT NUMBER: PREV200100449945
 TITLE: Antidiabetic properties of CLX-090700, a non-thiazolidinedione compound.
 AUTHOR(S): Gowri, Maya [Reprint author]; Dey, Deben [Reprint author]; Cheng, Jin [Reprint author]; Sen, Ananda [Reprint author]; **Medicherla, Satya** [Reprint author]; **Neogi, Partha** [Reprint author]
 CORPORATE SOURCE: Hayward, CA, USA
 SOURCE: Diabetes, (June, 2001) Vol. 50, No. Supplement 2, pp. A69. print.
 Meeting Info.: **61st Scientific Sessions of the American Diabetes Association**. Philadelphia, Pennsylvania, USA. June 22-26, 2001. American Diabetes Association.
 CODEN: DIAEAZ. ISSN: 0012-1797. ✓
 DOCUMENT TYPE: Conference; (Meeting)
 Conference; Abstract; (Meeting Abstract)
 LANGUAGE: English
 ENTRY DATE: Entered STN: 19 Sep 2001
 Last Updated on STN: 22 Feb 2002

L23 ANSWER 20 OF 20 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
 ACCESSION NUMBER: 1995:194325 BIOSIS
 DOCUMENT NUMBER: PREV199598208625
 TITLE: Co-regulation of very low density lipoprotein metabolism by dietary carbohydrate and cholesterol in hamsters.
 AUTHOR(S): Almario, R. [Reprint author]; **Medicherla, S.**; Kasim-Karakas, S. E.
 CORPORATE SOURCE: Univ. California, Davis, CA, USA
 SOURCE: FASEB Journal, (1995) Vol. 9, No. 3, pp. A440.
 Meeting Info.: Experimental Biology 95, Part I. Atlanta, Georgia, USA. April 9-13, 1995.
 CODEN: FAJOEC. ISSN: 0892-6638.
 DOCUMENT TYPE: Conference; (Meeting)
 Conference; Abstract; (Meeting Abstract)
 LANGUAGE: English
 ENTRY DATE: Entered STN: 5 May 1995
 Last Updated on STN: 15 May 1995

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2/4

Reyes 10/075,442

07/21/2004

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DICTIONARY FILE UPDATES: 19 JUL 2004 HIGHEST RN 713066-32-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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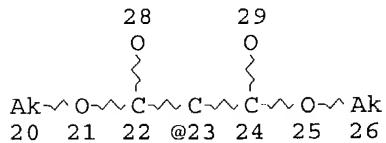
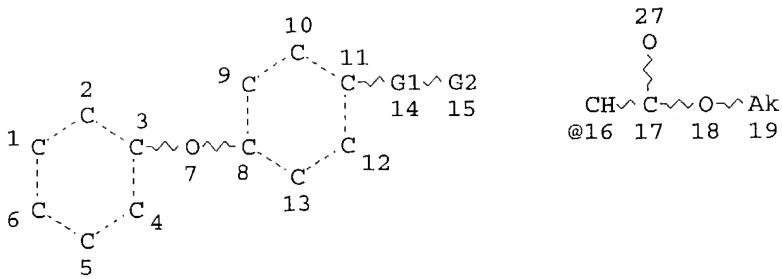
Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

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LAST RELOADED: Jul 16, 2004 (20040716/UP).

=> d que 118
L11 STR



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VAR G2=CH2/16/23

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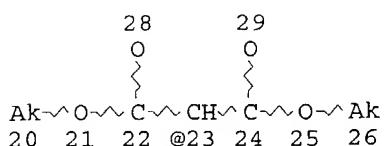
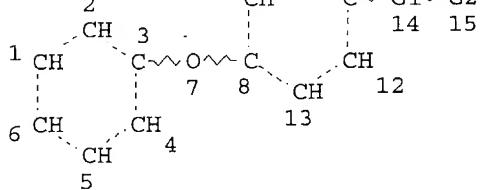
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CONNECT IS E1 RC AT 27
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE

L13 4813 SEA FILE=REGISTRY SSS FUL L11
L16 STR



VAR G1=CH2/16
VAR G2=CH3/32/23

NODE ATTRIBUTES:

NSPEC IS RC AT 7
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CONNECT IS E1 RC AT 28

CONNECT IS E1 RC AT 29
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE
L18 10 SEA FILE=REGISTRY SUB=L13 SSS FUL L16

=> fil reg

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STRUCTURE FILE UPDATES: 19 JUL 2004 HIGHEST RN 713066-32-1
DICTIONARY FILE UPDATES: 19 JUL 2004 HIGHEST RN 713066-32-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> analyze l18
ENTER ANSWER NUMBER OR RANGE (1-) :1-
ENTER DISPLAY CODE (CHEM) OR ?:lc
L20 ANALYZE L18 1- LC : 6 TERMS

=> d
L20 ANALYZE L18 1- LC : 6 TERMS

TERM #	# OCC	# DOC	% DOC	LC
1	10	10	100.00	CA
2	10	10	100.00	CAPLUS
3	4	4	40.00	BEILSTEIN
4	3	3	30.00	TOXCENTER
5	3	3	30.00	USPATFULL
6	2	2	20.00	CASREACT

***** END OF L20***

=> FIL STNGUIDE

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*** FILE CONTAINS 8,997,153 SUBSTANCES ***

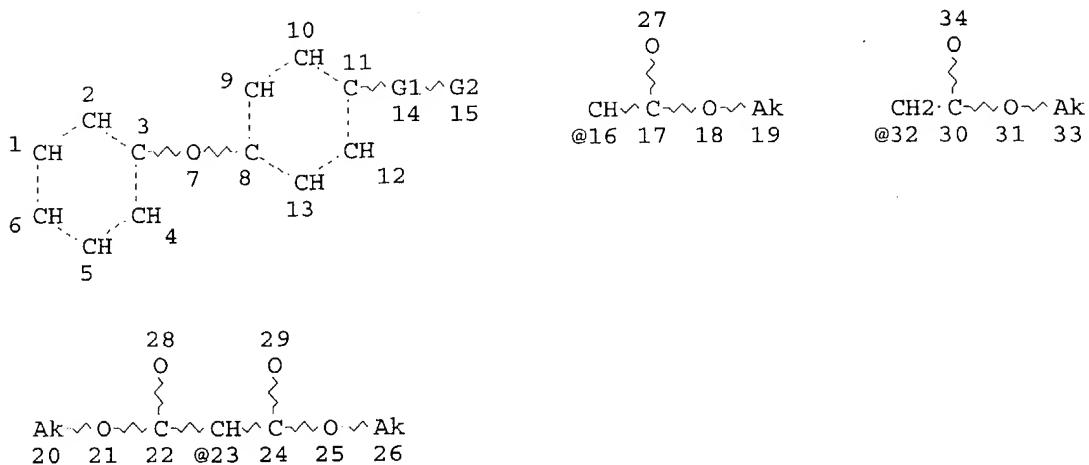
>>> PLEASE NOTE: Reaction data and substance data are stored in separate documents and can not be searched together in one query.

Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a molecular formula or a structure search for example can be restricted to compounds with available reaction information by concatenation with PRE/FA, REA/FA or more general with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be selected from substance answer sets and searched in the next step as reaction partner BRNs - Reactant (RX.RBRN) or Product BRN (RX.PBRN). After a search for reaction details substance documents associated with reactants or products may be retrieved by searching RX.PBRNs or RX.RBRNs as BRNs. <<<

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* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *

=> d que 122
L16 STR



VAR G1=CH2/16

VAR G2=CH3/32/23

NODE ATTRIBUTES:

NSPEC IS RC AT 7
 CONNECT IS E1 RC AT 27
 CONNECT IS E1 RC AT 28
 CONNECT IS E1 RC AT 29
 CONNECT IS E1 RC AT 34
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 34

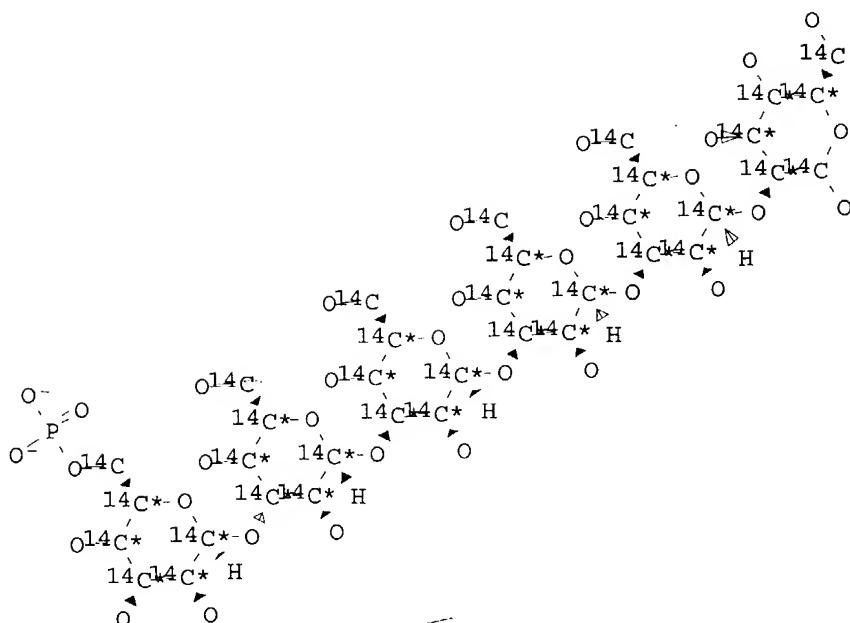
STEREO ATTRIBUTES: NONE

L21 8 SEA FILE=BEILSTEIN SSS FUL L16
 L22 4 SEA FILE=BEILSTEIN ABB=ON PLU=ON L21 NOT RN/FA

=> d ide l22

L22 ANSWER 1 OF 4 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN) :	9317926
Lin. Struct. Formula (LSF) :	(14)C36H61O34P(2-)
Molec. Formula (MF) :	C36 H61 O34 P
Molecular Weight (MW) :	1068.83
Lawson Number (LN) :	17647, 1122
File Segment (FS) :	Stereo compound
Compound Type (CTYPE) :	heterocyclic
Constitution ID (CONSID) :	7867777
Tautomer ID (TAUTID) :	8747803
Entry Date (DED) :	2003/04/17
Update Date (DUPD) :	2003/04/17



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
LSF	Linearized Structure Formula	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d 122 rx

L22 ANSWER 1 OF 4 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID) :	9208376
Reactant BRN (.RBRN) :	6409585
Reactant (.RCT) :	U-14C-Glucose
Product BRN (.PBRN) :	9315848, 9316930, 9317534, 9317926

Reyes 10/075,442

07/21/2004

Product (.PRO) : (14)C18H31O19P(2-) , (14)C24H41O24P(2-) ,
 (14)C30H51O29P(2-) , (14)C36H61O34P(2-)
 No. of React. Details (.NVAR) : 1

Reaction Details:

RX

Reaction RID (.RID) : 9208376.1
 Reaction Classification (.CL) : Multistage
 Nr. of Stages (.SNR) : 2
 Stage 1
 Reagent (.RGT) : Pichia hostii NRRL Y-2448 culture, KH2PO4
 Solvent (.SOL) : H2O
 Time (.TIM) : 15.5 hour(s)
 Temperature (.T) : 28 Cel
 Stage 2
 Reagent (.RGT) : HCl
 Solvent (.SOL) : H2O
 Time (.TIM) : 6 hour(s)
 pH Value (.PH) : 2
 Other Conditions (.COND) : Heating
 Note(s) (.COM) : Further byproducts given. Title compound
 not separated from byproducts

Reference(s):

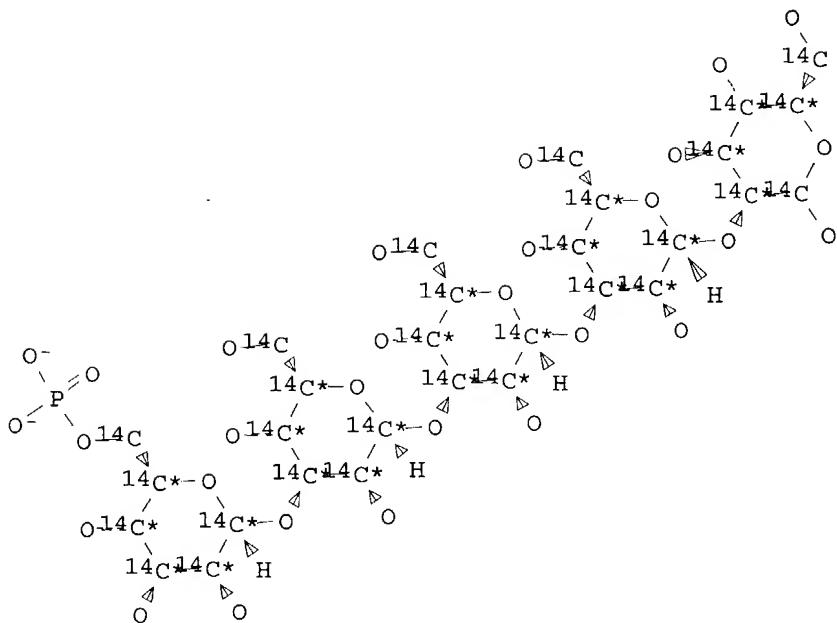
1. Ferro, Vito; Li, Caiping; Wang, Bin; Fewings, Kym; King, Andrew R.;
 Hammond, Edward; Creese, Brian R., J.Labelled Compd.Radiopharm., CODEN:
JLCRD4, 45(9), <2002>, 747 - 754; BABS-6369742

=> d l22 ide 2

MWSK

L22 ANSWER 2 OF 4 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN) : 9317534
 Lin. Struct. Formula (LSF) : (14)C30H51O29P(2-)
 Molec. Formula (MF) : C30 H51 O29 P
 Molecular Weight (MW) : 906.69
 Lawson Number (LN) : 17647, 1122
 File Segment (FS) : Stereo compound
 Compound Type (CTYPE) : heterocyclic
 Constitution ID (CONSID) : 7867414
 Tautomer ID (TAUTID) : 8747344
 Entry Date (DED) : 2003/04/17
 Update Date (DUPD) : 2003/04/17



Field Availability:

Code	Name	Occurrence
<hr/>		
BRN	Beilstein Records	1
LSF	Linearized Structure Formula	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
<hr/>		
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

d 122 rx 2

L22 ANSWER 2 OF 4 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID) : 9208376 *NPA*
 Reactant BRN (.RBRN) : 6409585
 Reactant (.RCT) : U-14C-Glucose

Product BRN (.PBRN) : 9315848, 9316930, 9317534, 9317926
 Product (.PRO) : (14)C18H31O19P(2-), (14)C24H41O24P(2-),
 (14)C30H51O29P(2-), (14)C36H61O34P(2-)
 No. of React. Details (.NVAR) : 1

Reaction Details:

RX

Reaction RID (.RID) : 9208376.1
 Reaction Classification (.CL) : Multistage
 Nr. of Stages (.SNR) : 2
 Stage 1
 Reagent (.RGT) : Pichia hostii NRRL Y-2448 culture, KH2PO4
 Solvent (.SOL) : H2O
 Time (.TIM) : 15.5 hour(s)
 Temperature (.T) : 28 Cel
 Stage 2
 Reagent (.RGT) : HCl
 Solvent (.SOL) : H2O
 Time (.TIM) : 6 hour(s)
 pH Value (.PH) : 2
 Other Conditions (.COND) : Heating
 Note(s) (.COM) : Further byproducts given. Title compound
 not separated from byproducts

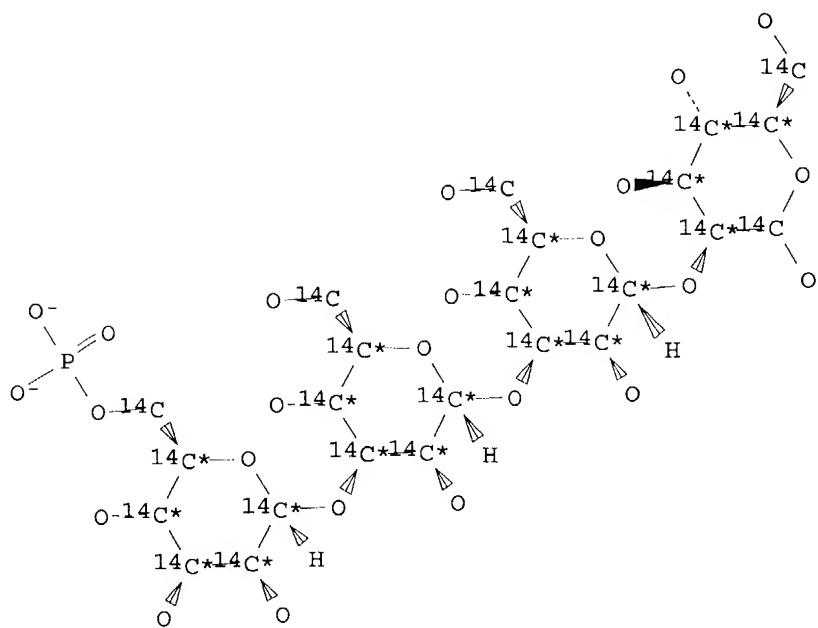
Reference(s):

1. Ferro, Vito; Li, Caiping; Wang, Bin; Fewings, Kym; King, Andrew R.;
 Hammond, Edward; Creese, Brian R., J.Labelled Compd.Radiopharm., CODEN:
 JLCRD4, 45(9), <2002>, 747 - 754; BABS-6369742

=> d 122 ide 3

L22 ANSWER 3 OF 4 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN) : 9316930
 Lin. Struct. Formula (LSF) : (14)C24H41O24P(2-)
 Molec. Formula (MF) : C24 H41 O24 P
 Molecular Weight (MW) : 744.55
 Lawson Number (LN) : 17647, 1122
 File Segment (FS) : Stereo compound
 Compound Type (CTYPE) : heterocyclic
 Constitution ID (CONSID) : 7866922
 Tautomer ID (TAUTID) : 8746329
 Entry Date (DED) : 2003/04/17
 Update Date (DUPD) : 2003/04/17



Field Availability:

Code	Name	Occurrence
<hr/>		
BRN	Beilstein Records	1
LSF	Linearized Structure Formula	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
<hr/>		
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

```
=>
=> d 122 rx 3
```

L22 ANSWER 3 OF 4 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

```
RX
  Reaction ID (.ID) : 9208376
  Reactant BRN (.RBRN) : 6409585
```

Reactant (.RCT) : U-14C-Glucose
 Product BRN (.PBRN) : 9315848, 9316930, 9317534, 9317926
 Product (.PRO) : (14)C18H31O19P(2-), (14)C24H41O24P(2-),
 (14)C30H51O29P(2-), (14)C36H61O34P(2-)
 No. of React. Details (.NVAR) : 1

Reaction Details:

RX

Reaction RID (.RID) : 9208376.1
 Reaction Classification (.CL) : Multistage
 Nr. of Stages (.SNR) : 2
 Stage 1
 Reagent (.RGT) : Pichia hostii NRRL Y-2448 culture, KH2PO4
 Solvent (.SOL) : H2O
 Time (.TIM) : 15.5 hour(s)
 Temperature (.T) : 28 Cel
 Stage 2
 Reagent (.RGT) : HCl
 Solvent (.SOL) : H2O
 Time (.TIM) : 6 hour(s)
 pH Value (.PH) : 2
 Other Conditions (.COND) : Heating
 Note(s) (.COM) : Further byproducts given. Title compound
 not separated from byproducts

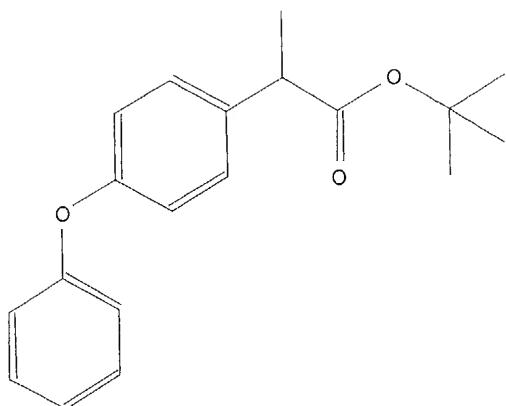
Reference(s) :
 1. Ferro, Vito; Li, Caiping; Wang, Bin; Fewings, Kym; King, Andrew R.;
 Hammond, Edward; Creese, Brian R., J.Labelled Compd.Radiopharm., CODEN:
 JLCRD4, 45(9), <2002> 747 - 754; BABS-6369742

=> d ide 122 4

L22 ANSWER 4 OF 4 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN) : 8984649
 Chemical Name (CN) : tert-butyl α -(4-diphenoxyl)propionate
 Autonom Name (AUN) : 2-(4-phenoxy-phenyl)-propionic acid
 tert-butyl ester

Molec. Formula (MF) : C19 H22 O3
 Molecular Weight (MW) : 298.38
 Lawson Number (LN) : 11705, 5219, 318
 Compound Type (CTYPE) : isocyclic
 Constitution ID (CONSID) : 7596317
 Tautomer ID (TAUTID) : 8448692
 Entry Date (DED) : 2002/04/29
 Update Date (DUPD) : 2002/04/29



Field Availability:

Code	Name	Occurrence
<hr/>		
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1
NMR	Nuclear Magnetic Resonance	3

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
<hr/>		
RX	Reaction Documents	2
RXPRO	Substance is Reaction Product	2

=> d rx l22 4

L22 ANSWER 4 OF 4 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID):	8938769
Reactant BRN (.RBRN):	1747857, 1948803
Reactant (.RCT):	propionic acid tert-butyl ester, (4-chloro-phenyl)-phenyl ether
Product BRN (.PBRN):	8984649
Product (.PRO):	2-(4-phenoxy-phenyl)-propionic acid tert-butyl ester
No. of React. Details (.NVAR):	1

Reaction Details:

RX

Reaction RID (.RID) : 8938769.1
 Reaction Classification (.CL) : Preparation
 Yield (.YDT) : 54 percent (BRN=8984649)
 Reagent (.RGT) : Pd₂(dba)₃, LiHMDS, 2-P(t-Bu)2-2'-NMe₂-1,1'-biphenyl
 Solvent (.SOL) : toluene
 Time (.TIM) : 3 hour(s)
 Temperature (.T) : 80 Cel
 Reference(s) :
 1. Moradi, Wahed A.; Buchwald, Stephen L., J.Amer.Chem.Soc., CODEN: *JACSAT*, 123(33), <2001>, 7996 - 8002; BABS-6324113

WPA

Reaction:

RX

Reaction ID (.ID) : 8934433
 Reactant BRN (.RBRN) : 1747857, 1308972
 Reactant (.RCT) : propionic acid tert-butyl ester,
 1-bromo-4-phenoxy-benzene
 Product BRN (.PBRN) : 8984649
 Product (.PRO) : 2-(4-phenoxy-phenyl)-propionic acid
 tert-butyl ester
 No. of React. Details (.NVAR) : 1

Reaction Details:

RX

Reaction RID (.RID) : 8934433.1
 Reaction Classification (.CL) : Preparation
 Yield (.YDT) : 71 percent (BRN=8984649)
 Reagent (.RGT) : Pd(OAc)₂, LiHMDS, 2-PCy₂-2'-NMe₂-1,1'-biphenyl
 Solvent (.SOL) : toluene
 Time (.TIM) : 2 hour(s)
 Temperature (.T) : 80 Cel
 Reference(s) :
 1. Moradi, Wahed A.; Buchwald, Stephen L., J.Amer.Chem.Soc., CODEN: *JACSAT*, 123(33), <2001>, 7996 - 8002; BABS-6324113

WPA

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=>

3/4
07/21/2004

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STRUCTURE FILE UPDATES: 19 JUL 2004 HIGHEST RN 713066-32-1
DICTIONARY FILE UPDATES: 19 JUL 2004 HIGHEST RN 713066-32-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

=> fil beilst

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FILE RELOADED ON OCTOBER 20, 2002
FILE LAST UPDATED ON JUNE 15, 2004

FILE COVERS 1771 TO 2003.
*** FILE CONTAINS 8,997,153 SUBSTANCES ***

>>> PLEASE NOTE: Reaction data and substance data are stored in
separate documents and can not be searched together in one
query.
Reaction data for BEILSTEIN compounds may be displayed
immediately with the display codes PRE (preparations) and REA
(reactions). A substance answer set retrieved after the search
for a chemical name, a molecular formula or a structure search
for example can be restricted to compounds with available
reaction information by concatenation with PRE/FA, REA/FA or
more general with RX/FA. The BEILSTEIN Registry Number (BRN)
is the link between a BEILSTEIN compound and belonging reactions.
For more detailed reaction searches BRNs can be selected from

substance answer sets and searched in the next step as reaction partner BRNs - Reactant (RX.RBRN) or Product BRN (RX.PBRN). After a search for reaction details substance documents associated with reactants or products may be retrieved by searching RX.PBRNs or RX.RBRNs as BRNs. <<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

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* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE, THESE *
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FILE COVERS 1907 - 20 Jul 2004 VOL 141 ISS 4
FILE LAST UPDATED: 19 Jul 2004 (20040719/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> fil uspatfull

FILE 'USPATFULL' ENTERED AT 15:11:42 ON 20 JUL 2004
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FILE COVERS 1971 TO PATENT PUBLICATION DATE: 20 Jul 2004 (20040720/PD)
FILE LAST UPDATED: 20 Jul 2004 (20040720/ED)
HIGHEST GRANTED PATENT NUMBER: US6766528
HIGHEST APPLICATION PUBLICATION NUMBER: US2004139525
CA INDEXING IS CURRENT THROUGH 20 Jul 2004 (20040720/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 20 Jul 2004 (20040720/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2004
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2004

>>> USPAT2 is now available. USPATFULL contains full text of the <<<
>>> original, i.e., the earliest published granted patents or <<<
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>>> publications, starting in 2001, for the inventions covered in <<<

>>> USPATFULL. A USPATFULL record contains not only the original published document but also a list of any subsequent publications. The publication number, patent kind code, and publication date for all the US publications for an invention are displayed in the PI (Patent Information) field of USPATFULL records and may be searched in standard search fields, e.g., /PN, /PK, etc.

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>>> USPATFULL and USPAT2 can be accessed and searched together through the new cluster USPATALL. Type FILE USPATALL to enter this cluster.

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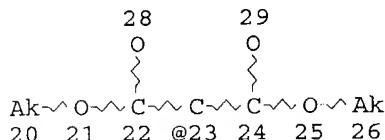
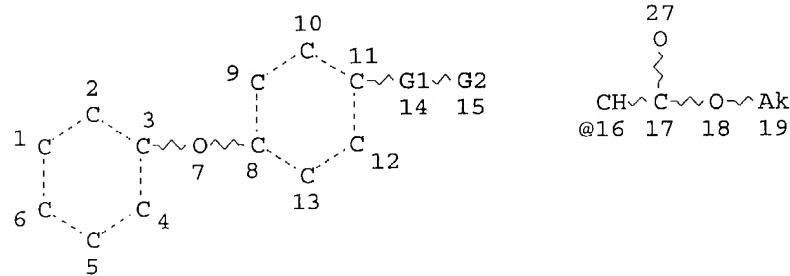
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LAST RELOADED: Jul 16, 2004 (20040716/UP).

=> d que 119

L11 STR



VAR G1=CH2/16
VAR G2=CH2/16/23
NODE ATTRIBUTES:
NSPEC IS RC AT 7
CONNECT IS E1 RC AT 27
CONNECT IS E1 RC AT 28
CONNECT IS E1 RC AT 29
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

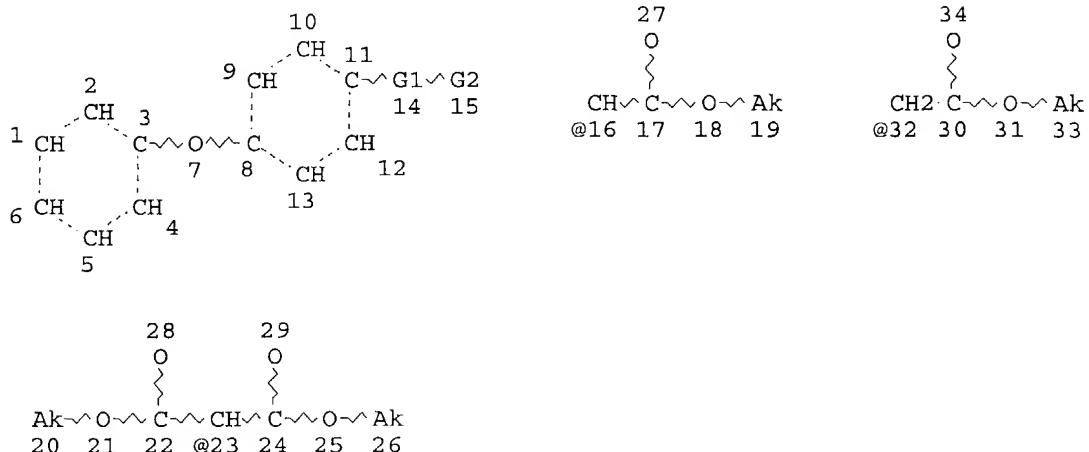
Reyes 10/075,442

07/21/2004

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE

L13 4813 SEA FILE=REGISTRY SSS FUL L11
L16 STR



VAR G1=CH2/16

VAR G2=CH3/32/23

NODE ATTRIBUTES:

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NODE ATTRIBUTES:
NSPEC IS RC AT 7
CONNECT IS E1 RC AT 27
CONNECT IS E1 RC AT 28
CONNECT IS E1 RC AT 29
CONNECT IS E1 RC AT 34
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMIT

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GRAPH ATTRIBUTES:

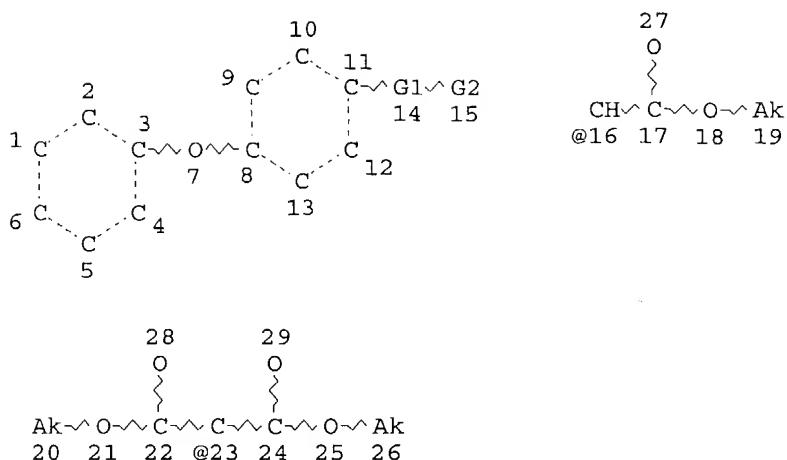
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE

L18 10 SEA FILE=REGISTRY SUB=L13 SSS FUL L16
L19 13 SEA FILE=HCAPLUS ABB=ON PLU=ON L18

=> d que 123
L11 STR



VAR G1=CH2/16
VAR G2=CH2/16/23

NODE ATTRIBUTES:

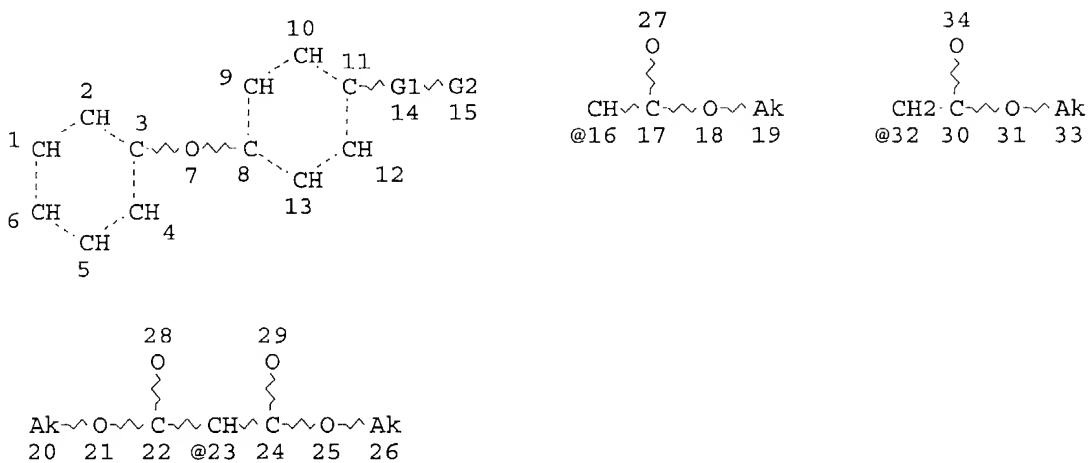
NSPEC IS RC AT 7
CONNECT IS E1 RC AT 27
CONNECT IS E1 RC AT 28
CONNECT IS E1 RC AT 29
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE

L13 4813 SEA FILE=REGISTRY SSS FUL L11
L16 STR



VAR G1=CH2/16
VAR G2=CH3/32/23

NODE ATTRIBUTES:

NSPEC IS RC AT 7
CONNECT IS E1 RC AT 27
CONNECT IS E1 RC AT 28

CONNECT IS E1 RC AT 29
 CONNECT IS E1 RC AT 34
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE
 L18 10 SEA FILE=REGISTRY SUB=L13 SSS FUL L16
 L23 2 SEA FILE=USPATFULL ABB=ON PLU=ON L18

=> dup rem 119 123

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 PROCESSING COMPLETED FOR L19
 PROCESSING COMPLETED FOR L23
 L24 15 DUP REM L19 L23 (0 DUPLICATES REMOVED)
 ANSWERS '1-13' FROM FILE HCAPLUS
 ANSWERS '14-15' FROM FILE USPATFULL

=> d iall hitstr 1-13

L24 ANSWER 1 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2001:546122 HCAPLUS
 DOCUMENT NUMBER: 135:257023
 ENTRY DATE: Entered STN: 29 Jul 2001
 TITLE: Palladium-catalyzed α -arylation of esters
 AUTHOR(S): Moradi, Wahed A.; Buchwald, Stephen L.
 CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
 SOURCE: Journal of the American Chemical Society (2001), 123(33), 7996-8002
 PUBLISHER: CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: American Chemical Society
 LANGUAGE: Journal
 CLASSIFICATION: English
 OTHER SOURCE(S): 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 ABSTRACT: CASREACT 135:257023

A new and simple one-pot procedure for the palladium-catalyzed intermol. α -arylation of esters is described. A number of esters, e.g. MeCO₂CMe₃, can be functionalized with a wide range of aryl bromides, e.g. 2-MeC₆H₄Br, using Pd(OAc)₂ or Pd₂(dba)₃ and bulky electron-rich o-biphenyl phosphines. Under the reaction conditions, using LiHMDS as base, α -arylation proceeds at room temperature or at 80°C with very good yields and high selectivities for monoarylation. Important nonsteroidal antiinflammatory drug derivs. such as (\pm)-naproxen tert-Bu ester and (\pm)-flurbiprofen tert-Bu ester can be prepared in 79% and 86% yield, resp. The catalyst system based on the o-biphenyl containing a dimethylamino group and di-tert-butylphosphine moiety is also active for the α -arylation of esters using aryl chlorides. Furthermore, using a

bipnaphthyl di-*tert*-butylphosphine ligand, the α -arylation of trisubstituted ester enolates can be accomplished to provide compds. that have quaternary centers.

SUPPL. TERM: arylation ester palladium biphenyl binaphthyl ligand catalyst

INDEX TERM: Arylation
Arylation catalysts
(palladium-catalyzed α -arylation of esters with aryl halides using biphenyl/binaphthyl phosphine ligands)

INDEX TERM: Aryl halides
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(palladium-catalyzed α -arylation of esters with aryl halides using biphenyl/binaphthyl phosphine ligands)

INDEX TERM: 3375-31-3, palladium(II) acetate 51364-51-3, Pd2(dba)3
213697-53-1 224311-49-3 224311-52-8
ROLE: CAT (Catalyst use); USES (Uses)
(palladium-catalyzed α -arylation of esters with aryl halides using biphenyl/binaphthyl phosphine ligands)

INDEX TERM: 92-66-0, 1-Bromo-4-phenylbenzene 95-46-5, 2-Bromotoluene
101-55-3, 1-Bromo-4-phenoxybenzene 101-97-3, Ethyl
2-phenylacetate 103-64-0, 1-Bromo-2-phenylethene
106-38-7, 4-Bromotoluene 106-43-4, 4-Chlorotoluene
108-37-2, 1-Bromo-3-chlorobenzene 401-78-5,
1-Bromo-3-(trifluoromethyl)benzene 460-00-4,
1-Bromo-4-fluorobenzene 540-88-5, tert-Butyl acetate
576-22-7, 1-Bromo-2,6-dimethylbenzene 580-13-2,
2-Bromonaphthalene 586-77-6, 1-Bromo-4-(dimethylamino)benzene 623-12-1, 1-Chloro-4-methoxybenzene
2039-88-5, 1-Bromo-2-vinylbenzene 2308-38-5, tert-Butyl
butanoate 5111-65-9, 2-Bromo-6-methoxynaphthalene
5892-99-9 7005-72-3, 1-Chloro-4-phenoxybenzene
7073-94-1, 1-Bromo-2-(isopropyl)benzene 7452-79-1, Ethyl
2-methylbutanoate 20487-40-5, tert-Butyl propanoate
23786-14-3 41604-19-7, 1,1'-Biphenyl, 4-bromo-2-fluoro
59247-47-1, tert-Butyl 4-bromobenzoate
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(palladium-catalyzed α -arylation of esters with aryl halides using biphenyl/binaphthyl phosphine ligands)

INDEX TERM: 5359-57-9P 5589-35-5P 33155-60-1P 62381-17-3P
63860-06-0P 68825-45-6P 93579-03-4P 124853-54-9P
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362523-57-7P 362523-58-8P
ROLE: SPN (Synthetic preparation); PREP (Preparation)
(palladium-catalyzed α -arylation of esters with aryl halides using biphenyl/binaphthyl phosphine ligands)

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD.

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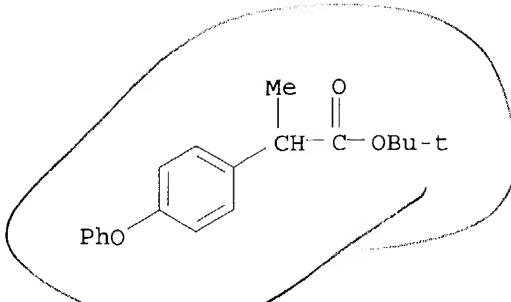
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IT 362523-48-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (palladium-catalyzed α -arylation of esters with aryl halides
 using biphenyl/binaphthyl phosphine ligands)

RN 362523-48-6 HCAPLUS

CN Benzeneacetic acid, α -methyl-4-phenoxy-, 1,1-dimethylethyl ester
 (9CI) (CA INDEX NAME)



NBA

L24 ANSWER 2 OF 15 HCPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2000:136796 HCPLUS
 DOCUMENT NUMBER: 132:265251
 ENTRY DATE: Entered STN: 29 Feb 2000
 TITLE: Synthesis of antiinflammatory analgesics
 bisphosphonate compounds
 AUTHOR(S): Zheng, Hu; Wu, Yong; Weng, Ling-Ling
 CORPORATE SOURCE: School of Pharmacy, West China University of Medical
 Sciences, Chengdu, 610041, Peop. Rep. China
 SOURCE: Hecheng Huaxue (1999) 07(4), 427-429
 PUBLISHER: Hecheng Huaxue Bianjibu
 DOCUMENT TYPE: Journal
 LANGUAGE: Chinese
 CLASSIFICATION: 29-7 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 1

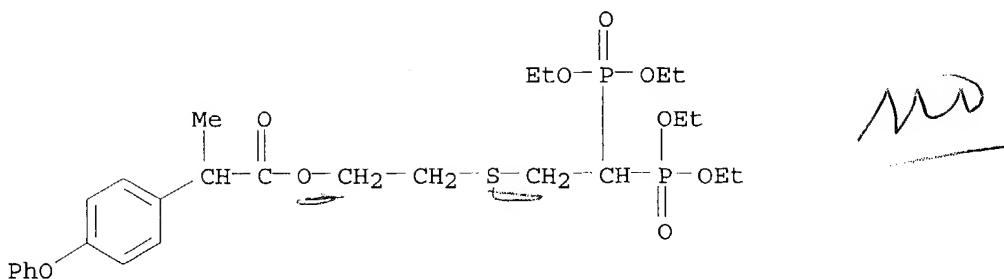
ABSTRACT:
 Bisphosphonates, e.g. HOCH₂CH₂SCH₂CH[P(O)(OEt)₂]₂, have bone-seeking affinity, antiarthritic and analgesic activity as well. In order to research bone-targeted leading compds. with high activity of antihypertrophic arthritics and low toxicity, five antiinflammatory analgesics-bisphosphonate compds. were designed and synthesized.

SUPPL. TERM: antiinflammatory analgesic bis phosphonate prep;
 bisphosphonate prep antiinflammatory analgesic
 INDEX TERM: Antiarthritics
 (antihypertrophic; synthesis of antiinflammatory
 analgesics bisphosphonate compds.)
 INDEX TERM: Anti-inflammatory agents
 (nonsteroidal; synthesis of antiinflammatory analgesics
 bisphosphonate compds.)
 INDEX TERM: 6145-33-1P 121001-81-8P 177172-94-0P 182919-44-4P
 263565-12-4P 263565-13-5P 263565-14-6P
 263565-15-7P 263565-16-8P 263565-17-9P
 ROLE: BAC (Biological activity or effector, except adverse);
 BSU (Biological study, unclassified); SPN (Synthetic
 preparation); BIOL (Biological study); PREP (Preparation)
 (synthesis of antiinflammatory analgesics bisphosphonate
 compds.)

IT 263565-15-7P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); SPN (Synthetic preparation); BIOL (Biological
 study); PREP (Preparation)
 (synthesis of antiinflammatory analgesics bisphosphonate compds.)

RN 263565-15-7 HCPLUS

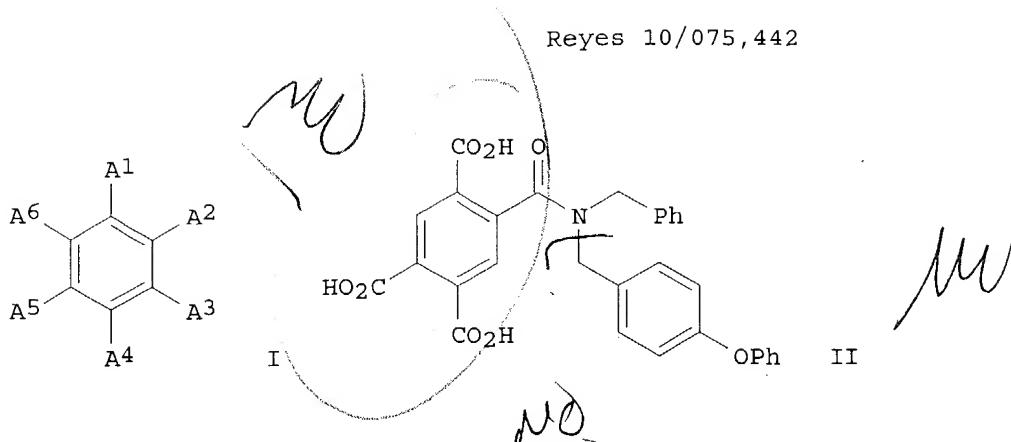
CN Benzeneacetic acid, α -methyl-4-phenoxy-, 2-[2,2-
 bis(diethoxyphosphinyl)ethyl]thio]ethyl ester (9CI) (CA INDEX NAME)



L24 ANSWER 3 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1997:44662 HCAPLUS
 DOCUMENT NUMBER: 126:59751
 ENTRY DATE: Entered STN: 22 Jan 1997
 TITLE: Preparation of di- and tricarboxybenzamides and
 analogs as squalene synthetase and protein
 farnesyltransferase inhibitors
 INVENTOR(S): Baker, William R.; Rosenberg, Saul H.; Fung, K. L.
 Anthony; Rockway, Todd W.; Fakhoury, Stephen A.;
 Garvey, David S.; Donner, B. Gregory; O'Connor,
 Stephen J.; Prasad, Rajnandan N.; Shen, Wang; Stout,
 David M.; Sullivan, Gerard M.
 PATENT ASSIGNEE(S): Abbott Laboratories, USA
 SOURCE: PCT Int. Appl., 241 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 INT. PATENT CLASSIF.:
 MAIN: C07C233-73
 SECONDARY: C07C233-65; C07C235-38; C07D257-04; C07C275-42;
 C07C335-22; C07C233-12; C07D333-20
 CLASSIFICATION: 25-19 (Benzene, Its Derivatives, and Condensed
 Benzenoid Compounds)
 Section cross-reference(s): 1
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9634851	A1	19961107	WO 1996-US6193	19960502
W: AU, CA, JP, KR, MX				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
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AU 9656731	A1	19961121	AU 1996-56731	19960502
PRIORITY APPLN. INFO.:			US 1995-429095	19950503
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			US 1993-147708	19931104
			US 1994-289711	19940909
			US 1994-322783	19941018
			WO 1996-US6193	19960502

OTHER SOURCE(S): MARPAT 126:59751
 GRAPHIC IMAGE:

**ABSTRACT:**

Title compds. [e.g., I; A₁ = ZCONR₁R₂, A₂, A₄, and A₅ or A₂ and A₄ or A₃ and A₄ = (protected) CO₂H and the other A_n = H; R₁ = (chloro)benzyl, (CH₂)₂-4Ph, CH₂C₆H₄(OPh)-4; R₂ = (CH₂)₁₋₂C₆H₄(OPh)-4; Z = bond, NR, O; R = H, (cyclo)alkyl, aralkyl, cycloalkylalkyl] were prepared. Thus, 4-(PhO)C₆H₄CHO was reductively aminated by H₂CH₂Ph and the product amidated by 1,2,4,5-benzenetetracarboxylic dianhydride to give title compound II. Data for in vitro inhibition of protein farnesyltransferase by selected I were given.

SUPPL. TERM: carboxybenzamide squalene synthetase protein
farnesyltransferase inhibitor

INDEX TERM: Artery, disease
(coronary, restenosis, prevention; preparation of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

INDEX TERM: Ras proteins
ROLE: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(farnesylation; preparation of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

INDEX TERM: Antitumor agents
(preparation of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

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 185050-25-3P 185051-65-4P

ROLE: BAC (Biological activity or effector, except adverse);
 BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

INDEX TERM:

131384-38-8, Protein farnesyltransferase

ROLE: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
 (preparation of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

INDEX TERM:

170433-63-3P, 1,2-Benzenedicarboxylic acid, 4-hydroxymethyl-, dimethyl ester

ROLE: BYP (Byproduct); PREP (Preparation)

(preparation of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

INDEX TERM:

61-54-1, 3-(2-Aminoethyl)indole 65-49-6, 4-Aminosalicylic acid 67-36-7, 4-Phenoxybenzaldehyde 85-44-9, 1,3-Isobenzofurandione 89-32-7 89-51-0, Homophthalic acid 89-57-6, 5-Aminosalicylic acid 89-93-0, 2-Methylbenzylamine 93-09-4, 2-Naphthoic acid 93-55-0, Propiophenone 95-48-7, reactions 95-65-8, 3,4-Dimethylphenol 96-32-2, Methyl bromoacetate 99-63-8, 1,3-Benzenedicarbonyl dichloride 100-20-9, 1,4-Benzenedicarbonyl dichloride 100-39-0, Benzyl bromide 100-46-9, Benzylamine, reactions 100-51-6, Benzyl alcohol,

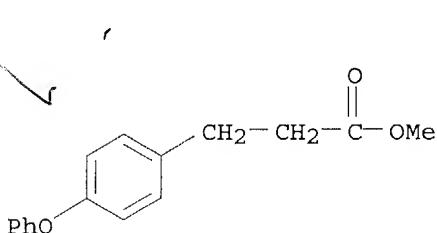
reactions 100-52-7, Benzaldehyde, reactions 100-81-2,
3-Methylbenzylamine 101-53-1, 4-Hydroxydiphenylmethane
103-49-1, Dibenzylamine 103-63-9, Phenethyl bromide
106-44-5, 4-Methylphenol, reactions 106-48-9,
4-Chlorophenol 108-39-4, 3-Methylphenol, reactions
118-31-0, 1-Naphthylmethylamine 138-25-0 150-76-5,
4-Methoxyphenol 459-57-4, 4-Fluorobenzaldehyde 527-60-6,
2,4,6-Trimethylphenol 552-30-7 556-56-9, Allyl iodide
569-51-7, 1,2,3-Benzenetricarboxylic acid 610-22-0,
Dimethyl 4-nitrophthalate 699-98-9, 2,3-
Pyridinedicarboxylic anhydride 703-59-3, Homophthalic
anhydride 1204-28-0, 4-Chlorocarbonylphthalic anhydride
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3-Nitroisophthalic acid monomethyl ester 2038-57-5,
Benzene propanamine 2045-79-6, 2-Methoxyphenethylamine
2217-40-5, 1-Amino-1,2,3,4-Tetrahydronaphthalene
2270-20-4, 5-Phenylpentanoic acid 2393-23-9,
4-Methoxybenzylamine 2420-87-3, [5,5'-Biisobenzofuran]-
1,1',3,3'-tetrone 2421-28-5 2426-87-1,
4-Benzyl oxy-3-methoxybenzaldehyde 2672-58-4,
1,3,5-Benzenetricarboxylic acid, trimethyl ester
2687-43-6, O-Benzylhydroxylamine hydrochloride 2740-83-2,
3-Trifluoromethylbenzylamine 2835-06-5 2975-41-9,
2-Aminoindane 3048-01-9, 2-Trifluoromethylbenzylamine
3082-77-7, L-Methionine ethyl ester 3113-72-2,
5-Methyl-2-nitrobenzoic acid 3132-99-8,
3-Bromobenzaldehyde 3218-02-8, Cyclohexanemethanamine
3218-36-8, 4-Phenylbenzaldehyde 3669-48-5 3711-01-1,
2,3,6,7-Naphthalenetetracarboxylic dianhydride 3731-51-9,
2-Pyridylmethylamine 3731-52-0, 3-Pyridylmethylamine
3731-53-1, 4-Pyridylmethylamine 3939-09-1,
2,4-Difluorobenzonitrile 4360-51-4, 1-Amino-3-phenyl-2-
propene 4393-09-3, 2,3-Dimethoxybenzylamine 4397-53-9,
4-Benzyl oxybenzaldehyde 4442-59-5, 1,4-Benzodioxan-2-
methylamine 4821-94-7, 4,5-Dimethoxyphthalic anhydride
5326-47-6, 2-Amino-5-iodobenzoic acid 5372-81-6, Dimethyl
aminoterephthalate 5470-84-8, 4-Benzyl oxybutyraldehyde
5736-88-9, 4-Butoxybenzaldehyde 5870-38-2, Diethyl
2,5-dihydroxyterephthalate 5927-18-4,
Trimethylphosphonoacetate 6050-13-1, Diphenic anhydride
6287-38-3, 3,4-Dichlorobenzaldehyde 6328-74-1,
4-Phenoxyphenylacetic acid 6850-57-3, 2-Methoxybenzylamine
6921-34-2, Benzylmagnesium chloride 7355-22-8,
5-Bromo-2,4-dihydroxybenzoic acid 7409-30-5,
4-Nitrobenzylamine 7617-76-7, 3-Phenoxypropylamine
7745-93-9, 2-Bromo-4-nitrotoluene 13214-66-9,
4-Phenylbutylamine 17532-66-0, 1,2-Benzenediacetic acid,
diethyl ester 18655-51-1, 3-(2-Methoxyphenyl)propylamine
19014-14-3 19434-34-5, 2-Phenoxybenzaldehyde 20116-65-8,
Dimethyl 4-methylphthalate 20781-22-0 22117-85-7
22440-62-6 22479-95-4, Dimethyl 4-hydroxyphthalate
24541-01-3, 4-Chromanone oxime 24850-33-7,
Allyltributyltin 26759-46-6 27757-85-3,
2-Thiophenemethanamine 28994-41-4, 2-
Hydroxydiphenylmethane 34698-41-4, 1-Aminoindane
37806-29-4, 2-Ethoxybenzylamine 37806-49-8,
Benzene methanamine, 2-(3-methylbutoxy)- 37806-66-9
39515-51-0, 3-Phenoxybenzaldehyde 39590-27-7,
Benzeneethanamine, 2-ethoxy- 40663-68-1,
4-Allyloxybenzaldehyde 42116-44-9, N-tert-

Butoxycarbonylbenzenemethanamine 58332-00-6 60728-41-8
 69770-20-3, 3-(4-Chlorophenoxy)benzaldehyde 69770-23-6,
 3-(4-tert-Butylphenoxy)benzaldehyde 72235-53-1,
 3,4-Difluorobenzylamine 79124-75-7, 3-(4-Methylphenoxy)benzaldehyde 79124-76-8,
 3-(3,4-Dichlorophenoxy)benzaldehyde 88088-95-3,
 Tris(1-benzotriazolyl)methane 107624-14-6,
 Benzenemethanamine, 2-phenoxy- 165534-79-2, Dimethyl iodoterephthalate 169943-62-8 169943-64-0 171350-07-5
 171350-08-6 184229-19-4, 4-Phenoxy-3-chlorobenzaldehyde 185051-61-0 185051-62-1 185051-63-2 185051-64-3,
 N-Benzyl-2-fluorenethylmethylamine
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

INDEX TERM:
 2215-84-1P 3786-39-8P 3898-66-6P 4315-09-7P,
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 19241-40-8P 20116-67-0P, 1,2-Benzenedicarboxylic acid,
 4-bromomethyl-, dimethyl ester 29710-58-5P 38588-64-6P,
 1,3,5-Benzenetricarboxylic acid, dimethyl ester 39585-32-5P, Benzeneacetic acid, 2-carboxy-5-nitro-40172-06-3P, N-(3,4-Dichlorobenzyl)ethanolamine 46253-86-5P 51832-31-6P, Dimethyl 4-aminophthalate 52446-51-2P, 2-(4-Phenoxyphenyl)ethanol 53981-38-7P,
 4-Aminochroman 60313-18-0P 63746-12-3P, Dimethyl 4-aminoisophthalate 64481-29-4P 67402-72-6P
 68872-14-0P 69048-70-0P, Dimethyl 4-nitroisophthalate 74733-34-9P 76784-89-9P, Benzeneacetic acid,
 5-amino-2-(methoxycarbonyl)-, methyl ester 79807-86-6P
 91345-28-7P 91963-85-8P 100959-22-6P, Methyl 2-bromo-4-nitrobenzoate 110786-89-5P, 1,2-Benzenedicarboxylic acid, 4-mercaptop-, dimethyl ester 129951-06-0P, Benzenebutanamine, N-phenylmethyl-136534-67-3P, Benzenepentanamine, N-phenylmethyl-138408-68-1P, Methyl 4-hydroxy-2-methoxy-5-vinylbenzoate 144146-84-9P, N-Benzyl-5-phenylPantanamide 147810-06-8P
 169943-97-9P, N-Benzyl-N-(4-phenoxybenzyl)amine 170433-65-5P, Dimethyl 4-(carboxymethyl)phthalate 179056-63-4P 179098-29-4P 184033-42-9P,
 4-tert-Butoxycarbonylamino-2-hydroxyBenzoic acid 184228-76-0P 184228-77-1P 184228-78-2P 184228-79-3P
 185050-26-4P 185050-27-5P 185050-28-6P 185050-29-7P
 185050-30-0P 185050-31-1P 185050-32-2P,
 2-Cyano-5-iodobenzoic acid 185050-33-3P 185050-34-4P
 185050-35-5P 185050-36-6P 185050-37-7P 185050-38-8P
 185050-39-9P 185050-40-2P 185050-41-3P 185050-42-4P
 185050-43-5P 185050-44-6P 185050-45-7P 185050-46-8P
 185050-47-9P 185050-48-0P 185050-49-1P 185050-50-4P
 185050-51-5P 185050-52-6P 185050-53-7P 185050-54-8P
 185050-55-9P 185050-56-0P 185050-57-1P 185050-58-2P
 185050-59-3P 185050-60-6P 185050-61-7P 185050-62-8P
 185050-63-9P 185050-64-0P 185050-65-1P 185050-66-2P
 185050-67-3P 185050-68-4P 185050-69-5P 185050-70-8P
 185050-71-9P 185050-72-0P 185050-73-1P 185050-74-2P
 185050-75-3P 185050-76-4P 185050-77-5P, Methyl 5-bromo-4-hydroxy-2-methoxybenzoate 185050-78-6P
 185050-79-7P, Methyl 2-methoxy-4,5-divinylbenzoate 185050-80-0P, 2-Methoxy-4,5-divinylbenzoic acid 185050-81-1P 185050-82-2P 185050-83-3P 185050-84-4P

185050-85-5P 185050-86-6P 185050-87-7P 185050-88-8P
 185050-89-9P 185050-90-2P 185050-91-3P 185050-92-4P
 185050-93-5P 185050-94-6P, Methyl 4-tert-Butoxycarbonylamino-2-hydroxyBenzoate 185050-95-7P
 185050-96-8P 185050-97-9P 185050-98-0P 185050-99-1P
185051-00-7P 185051-01-8P **185051-02-9P**
 185051-03-0P 185051-04-1P 185051-05-2P 185051-06-3P
 185051-07-4P 185051-08-5P 185051-09-6P 185051-10-9P
 185051-11-0P 185051-12-1P 185051-13-2P 185051-14-3P
 185051-15-4P 185051-16-5P 185051-17-6P 185051-18-7P
 185051-19-8P 185051-20-1P 185051-21-2P 185051-22-3P
 185051-23-4P 185051-24-5P 185051-25-6P 185051-26-7P
 185051-27-8P 185051-28-9P 185051-29-0P 185051-30-3P
 185051-31-4P 185051-32-5P 185051-33-6P 185051-34-7P
 185051-35-8P 185051-36-9P 185051-37-0P 185051-38-1P
 185051-39-2P 185051-40-5P 185051-41-6P 185051-42-7P
 185051-43-8P 185051-44-9P 185051-45-0P 185051-46-1P
 185051-47-2P 185051-48-3P 185051-49-4P 185051-50-7P
 185051-51-8P 185051-52-9P 185051-53-0P 185051-54-1P
 185051-55-2P 185051-56-3P 185051-57-4P 185051-58-5P
 185051-59-6P 185051-60-9P 185051-67-6P 185230-57-3P
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

IT 185051-02-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)
 RN 185051-02-9 HCAPLUS
 CN Benzenepropanoic acid, 4-phenoxy-, methyl ester (9CI) (CA INDEX NAME)



L24 ANSWER 4 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1994:442116 HCAPLUS
 DOCUMENT NUMBER: 121:42116
 ENTRY DATE: Entered STN: 23 Jul 1994
 TITLE: Study on the source of nonvolatile mutagenic organics
 in the water of East Lake and the tap water from it
 AUTHOR(S): Tian, Shizhong; Huang, Zhidan; Deng, Nansheng; Zhang,
 Jiayao; Zhao, Pihong; Xiao, Mei; Liu, Dazhi; Zhizhong,
 Jing; Meilan, Wang; Xizhao, Yuan
 CORPORATE SOURCE: Dep. Environ. Sci., Wuhan Univ., Wuhan, 430072, Peop.
 Rep. China
 SOURCE: Zhongguo Huanjing Kexue (1993), 13(2), 100-5
 CODEN: ZHKEEI; ISSN: 1000-6923
 DOCUMENT TYPE: Journal
 LANGUAGE: Chinese
 CLASSIFICATION: 61-2 (Water)

Section cross-reference(s): 4, 10

ABSTRACT:

A total of 102 organic pollutants (alkylbenzenes, polycyclic aromatic hydrocarbons, phthalic esters, etc.) in East Lake and the tap water from it were identified by gas chromatog.-mass spectrometry. Ames test results showed that they have mutagenicity to TA98, and are direct mutagens. Model test of chlorination of humic acid or fulvic acid showed that humics of low concentration in water do not form nonvolatile mutagenic orgs. and nonvolatile mutagenic orgs. in the tap water from East Lake.

SUPPL. TERM: org water pollution East Lake China; *Salmonella typhimurium* toxicity org lake pollution; Ames test toxicity org water pollution

INDEX TERM: Water pollution
(by organic compds., of lake water and potable water,
Salmonella typhimurium toxicity in relation to, of East Lake, China)

INDEX TERM: Organic compounds, biological studies
ROLE: BIOL (Biological study)
(lake water and potable water pollution by, *Salmonella typhimurium* toxicity in relation to, of East Lake, China)

INDEX TERM: Toxicity
(of organic compds. in polluted lake water and potable water, to *Salmonella typhimurium* strain TA-98, Ames test determination of, of East Lake, China)

INDEX TERM: *Salmonella typhimurium*
(strain TA-98, polluted lake and potable water toxicity to, Ames test for, of East Lake, China)

INDEX TERM: 57-10-3, Hexadecanoic acid, biological studies 64-19-7, Acetic acid, biological studies 67-66-3, Trichloromethane, biological studies 71-43-2, Benzene, biological studies 75-27-4, Bromodichloromethane 75-65-0, Tert-Butanol, biological studies 84-66-2, Diethyl phthalate 84-69-5, Diisobutyl phthalate 84-74-2, Dibutyl phthalate 86-73-7, Fluorene 91-20-3, Naphthalene, biological studies 95-16-9, Benzothiazole 95-50-1, o-Dichlorobenzene 100-41-4, Ethylbenzene, biological studies 100-42-5, biological studies 100-52-7, Benzaldehyde, biological studies 106-46-7, p-Dichlorobenzene 108-88-3, Toluene, biological studies 108-90-7, Chlorobenzene, biological studies 110-54-3, Hexane, biological studies 110-82-7, Cyclohexane, biological studies 110-93-0, 6-Methyl-5-heptene-2-one 111-27-3, Hexanol, biological studies 111-65-9, Octane, biological studies 111-84-2, Nonane 112-30-1, Decanol 112-95-8, Eicosane 117-81-7, Dioctyl phthalate 120-12-7, Anthracene, biological studies 124-48-1, Dibromochloromethane 128-37-0, 2,6-Ditert-butyl-4-methylphenol, biological studies 128-39-2, 2,6-Di-tert-butylphenol 131-11-3 140-29-4, Benzylcyanide 206-44-0, Fluoranthene 486-25-9, 9H-Fluoren-9-one 489-84-9 535-77-3, 1-Methyl-3-isopropylbenzene 541-73-1, m-Dichlorobenzene 544-63-8, Tetradecanoic acid, biological studies 593-45-3, Octadecane 629-78-7, Heptadecane 629-92-5, Nonadecane 629-94-7, Heneicosane 629-97-0, Docosane 646-31-1, Tetracosane 678-26-2, Perfluoropentane 719-22-2 763-93-9, 3-Hexen-2-one 814-78-8 934-34-9, Benzothiazolone 937-30-4 1138-52-9, 3,5-Di-tert-butylphenol 1331-43-7, Diethylcyclohexane 1569-50-2,

3-Pentene-2-ol 1689-78-7, 2-tert-Butylthiophene
 2142-64-5 2219-82-1, 2-tert-Butyl-6-methylphenol
 2245-30-9 2444-28-2, 2,6-Di-tert-butyl-1,4-benzenediol
 4130-42-1, 2,6-Di-tert-butyl-4-ethylphenol 4281-40-7
 4562-27-0, 4-(1H)-Pyrimidinone 4675-87-0 4920-99-4,
 1-Ethyl-3-isopropylbenzene 7507-89-3 11071-47-9,
 Isooctene 12002-48-1, Trichlorobenzene 15356-74-8
 18794-47-3 19377-95-8 24270-68-6, 1,1,2,3-
 Tetrafluoropropane 25377-83-7, Octene 25378-22-7,
 Dodecene 25495-91-4, Bromohexane 27138-19-8,
 Ethylnaphthalene 27195-67-1, Dimethylcyclohexane
 27400-77-7, Nonadecene 27400-79-9, Heneicosene
 28351-09-9, Dimethylbenzaldehyde 28804-88-8,
 Dimethylnaphthalene 29253-36-9, Isopropylnaphthalene
 29512-02-5, 1-Methoxy-1-butene 29730-67-4, Docosene
 34314-83-5, 4-Methyl-2,3-dihydrofuran 34464-40-9,
 Isononane 34970-00-8, Iodobromochloromethane
36207-23-5 53951-50-1, Ethylbenzaldehyde
 58501-92-1 61923-54-4, 2-Penten-2-ol 62808-70-2
 103502-85-8 156000-89-4 156057-47-5
 ROLE: BIOL (Biological study)
 (lake water and potable water pollution by, *Salmonella typhimurium* toxicity in relation to, of East Lake, China)

IT **36207-23-5**

RL: BIOL (Biological study)

(lake water and potable water pollution by, *Salmonella typhimurium* toxicity in relation to, of East Lake, China)

RN 36207-23-5 HCAPLUS

CN Benzene, 1-ethyl-4-phenoxy- (9CI) (CA INDEX NAME)



L24 ANSWER 5 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1990:206735 HCAPLUS
 DOCUMENT NUMBER: 112:206735
 ENTRY DATE: Entered STN: 26 May 1990
 TITLE: Preparation of α -arylacetic acid derivatives by electrochemical oxidation
 INVENTOR(S): Shono, Tatsuya; Matsumura, Isahiro
 PATENT ASSIGNEE(S): Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 INT. PATENT CLASSIF.:
 MAIN: C25B003-02
 CLASSIFICATION: 72-9 (Electrochemistry)
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01222078	A2	19890905	JP 1988-50233	19880302

PRIORITY APPLN. INFO.:

JP 1988-50233

19880302

OTHER SOURCE(S):

MARPAT 112:206735

ABSTRACT:

A method for preparing $AC_6H_5COOR_2$ ($A = \text{aryl}$, (condensed) heterocyclic group, $R, R_1 = \text{H}$, alkyl, alicyclic group, unsatd. hydrocarbon group, aryl, aralkyl; $R_2 = \text{H}$ or lower alkyl) involves electrochem. oxidation of $ACOCH_3R_1$ in the presence of I (or its compound) and an acetalization agent.

SUPPL. TERM: arylacetic acid prepn electrochem oxidn ketone

INDEX TERM: Oxidation, electrochemical

(of ketones, in preparation of arylacetic acid derivs.)

INDEX TERM: 74-88-4, uses and miscellaneous 149-73-5 7553-56-2, Iodine, uses and miscellaneous

ROLE: PROC (Process)

(electrochem. oxidation of ketones in presence of, for preparation of arylacetic acid derivs.)

INDEX TERM: 75-30-9 75-47-8 591-50-4 3240-34-4 7553-56-2, Iodine, uses and miscellaneous 7681-11-0, Potassium iodide (KI), uses and miscellaneous 7758-05-6 10034-85-2, Hydriodic acid 12027-06-4, Ammonium iodide ((NH₄)I) 16029-98-4

ROLE: PROC (Process)

(electrochem. oxidation of ketones in presence of, in preparation of arylacetic acid derivs.)

INDEX TERM: 93-55-0 98-86-2, reactions 495-40-9 582-62-7 611-70-1 712-50-5 889-26-9 1515-95-3 2700-47-2 6315-96-4 10342-83-3 52129-98-3 59771-24-3 66952-37-2 80336-83-0 114012-26-9 120703-45-9 126916-32-3 126934-92-7 126934-93-8

ROLE: RCT (Reactant); RACT (Reactant or reagent)

(electrochem. oxidation of, in preparation of arylacetic acid derivs.)

INDEX TERM: 101-41-7P 2294-71-5P 17380-78-8P 30012-51-2P 31508-44-8P 50415-73-1P 52263-88-4P 57421-64-4P 57625-74-8P 59235-36-8P 61566-34-5P 66202-87-7P 72615-27-1P 73913-50-5P 83636-46-8P 103392-12-7P 120703-46-0P 125670-62-4P 126934-94-9P 126934-95-0P 126934-96-1P

ROLE: PREP (Preparation)

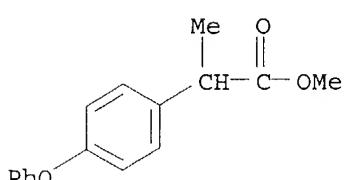
(preparation of, electrochem., by oxidation of ketone derivs.)

IT 126934-95-0P

RL: PREP (Preparation)

(preparation of, electrochem., by oxidation of ketone derivs.)

RN 126934-95-0 HCAPLUS

CN Benzeneacetic acid, α -methyl-4-phenoxy-, methyl ester (9CI) (CA INDEX NAME)

DOCUMENT NUMBER:

112:97962

ENTRY DATE:

Entered STN: 18 Mar 1990

TITLE:

Reactivity of ring-substituted ethylbenzenes in reactions with cumylperoxy radicals

AUTHOR(S):

Efimova, I. V.; Matvienko, A. G.; Opeida, I. A.

CORPORATE SOURCE:

Inst. Fiz.-Org. Khim. Uglekhim., Donetsk, USSR

SOURCE:

Zhurnal Organicheskoi Khimii (1989), 25(4), 801-4

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

CLASSIFICATION:

22-13 (Physical Organic Chemistry)

ABSTRACT:

The reaction constant ρ_+ [determined from σ_+ substituent consts. in $p\text{-RC}_6\text{H}_4\text{Et}$ (I)] for the H-abstraction reaction with $\text{PhCMe}_2\text{OO}\cdot$ was more statistically reliable than ρ , reflecting the significant contribution of polar conjugation of R with the reaction center in transition-state stabilization. The absolute magnitude of ρ_+ , on the basis of current and literature evaluations, decreased in the series $\text{RC}_6\text{H}_4\text{Me} > \text{I} > \text{RC}_6\text{H}_4\text{CHMe}_2$, reflecting the Hammond reactivity-selectivity principle.

SUPPL. TERM: abstraction hydrogen ethylbenzene deriv kinetics;
 substituent effect hydrogen abstraction ethylbenzene;
 reaction const hydrogen abstraction ethylbenzene; benzene
 alkyl reactivity selectivity

INDEX TERM: Reaction constant
 (for abstraction reaction of hydrogen from ethylbenzene
 derivs. with cumylperoxy radical)

INDEX TERM: Kinetics of abstraction reaction
 (of hydrogen, from ethylbenzene derivs. with cumylperoxy
 radical)

INDEX TERM: Substituent effect
 (on abstraction reaction of hydrogen from ethylbenzene
 derivs. with cumylperoxy radical)

INDEX TERM: 141-93-5, m-Diethylbenzene 937-30-4, p-Acetylethylbenzene
 1515-95-3, p-Methoxyethylbenzene 1585-07-5,
 p-Bromoethylbenzene 36207-23-5

ROLE: PRP (Properties)
 (abstraction reaction of hydrogen of, with cumylperoxy
 radical, kinetics of)

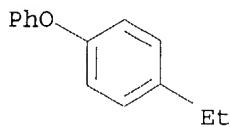
INDEX TERM: 7175-54-4, Cumylperoxy radical
 ROLE: PRP (Properties)
 (abstraction reaction of hydrogen of, with ethylbenzene
 derivs., kinetics of)

IT 36207-23-5

RL: PRP (Properties)
 (abstraction reaction of hydrogen of, with cumylperoxy radical,
 kinetics of)

RN 36207-23-5 HCPLUS

CN Benzene, 1-ethyl-4-phenoxy- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1989:231286 HCPLUS
 DOCUMENT NUMBER: 110:231286
 ENTRY DATE: Entered STN: 25 Jun 1989
 TITLE: Process for the preparation of 2-(substituted phenyl)propionates as pharmaceuticals or their intermediates
 INVENTOR(S): Takahashi, Eiji; Ozaki, Kazuo; Yamada, Takao
 PATENT ASSIGNEE(S): Maruzen Petrochemical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 INT. PATENT CLASSIF.: C07C059-64
 MAIN: B01J031-22; C07C051-14; C07C067-38; C07C069-734
 SECONDARY:
 CLASSIFICATION: 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 Section cross-reference(s): 1
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63290842	A2	19881128	JP 1987-125684	19870525
PRIORITY APPLN. INFO.:			JP 1987-125684	19870525

OTHER SOURCE(S): MARPAT 110:231286

ABSTRACT:

Title compds. R₁OC₆H₄CHMeCO₂R₂ (R₁ = Ph, Me; R₂ = H, alkyl), e.g. phenopropylene, are prepared by dehydrogenation of R₁OC₆H₄Et in the presence of a dehydrogenation catalyst at 400-700° and carbonylation of the resultant R₁OC₆H₄CH:CH₂ in H₂O or an alc. in the presence of a Pd catalyst. 3-PhOC₆H₄Et and H₂O at 0.5 h-1 LHSV were charged in a reactor containing tin oxide at 580°, to give 3-PhOC₆H₄CH:CH₂ in 61.3% yield, and the product was autoclaved with Me₂CHOH, PdCl₂(PPh₃)₂, PPh₃, and 35% HCl at 110° and 120 kg/cm² CO to give total 99.8% yield of 3-PhOC₆H₄CHMeCO₂CHMe₂ and 3-PhOC₆H₄(CH₂)₂CO₂CHMe₂ (93.2% and 6.4% selectivity, resp.).

SUPPL. TERM: phenylpropionate prepn pharmaceutical intermediate
 INDEX TERM: Pharmaceuticals
 (intermediates for, phenylpropionates as)
 INDEX TERM: Alkoxy carbonylation
 (of styrene derivs., phenylpropionates from)
 INDEX TERM: 1515-95-3, 4-Methoxyphenylethane 10568-38-4,
 3-Methoxyphenylethane 36207-23-5,
 4-Phenoxyphenylethane 78427-95-9, 3-Phenoxyphenylethane
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (dehydrogenation of, styrene derivative from)
 INDEX TERM: 4973-29-9P, 4-Phenoxyphenylethylene 10568-38-4P,
 3-Methoxyphenylethane 78427-95-9P, 3-Phenoxyphenylethane
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (preparation and alkoxy carbonylation of)
 INDEX TERM: 637-69-4P, 4-Methoxyphenylethylene
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (preparation and alkoxy carbonylation of)
 INDEX TERM: 113777-15-4P, Isopropyl 3-(3-methoxyphenyl)propionate
 120824-59-1P, Isopropyl 3-(3-phenoxyphenyl)propionate
 120824-60-4P, sec-Butyl 3-(4-phenoxyphenyl)propionate 120824-61-5P, sec-Butyl

3-(4-methoxyphenyl)propionate
 ROLE: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

INDEX TERM:

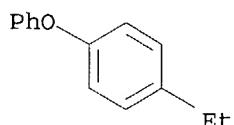
120824-55-7P, Isopropyl 2-(3-phenoxyphenyl)propionate
 120824-56-8P, sec-Butyl 2-(3-phenoxyphenyl)propionate
 120824-57-9P, sec-Butyl 2-(4-methoxyphenyl)propionate
 120824-58-0P, Isopropyl 2-(3-methoxyphenyl)propionate
 ROLE: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as intermediate for drugs)

IT 36207-23-5, 4-Phenoxyphenylethane

RL: RCT (Reactant); RACT (Reactant or reagent)
 (dehydrogenation of, styrene derivative from)

RN 36207-23-5 HCPLUS

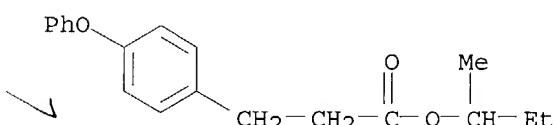
CN Benzene, 1-ethyl-4-phenoxy- (9CI) (CA INDEX NAME)



IT 120824-60-4P, sec-Butyl 3-(4-phenoxyphenyl)propionate
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 120824-60-4 HCPLUS

CN Benzenepropanoic acid, 4-phenoxy-, 1-methylpropyl ester (9CI) (CA INDEX NAME)



L24 ANSWER 8 OF 15 HCPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1989:594298 HCPLUS

DOCUMENT NUMBER: 111:194298

ENTRY DATE: Entered STN: 25 Nov 1989

TITLE: Preparation of substituted phenylpropionaldehydes as drug intermediates

INVENTOR(S): Takahashi, Eiji; Ozaki, Kazuo; Yamada, Takao

PATENT ASSIGNEE(S): Maruzen Petrochemical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

INT. PATENT CLASSIF.:

MAIN: C07C047-277

SECONDARY: C07C045-50

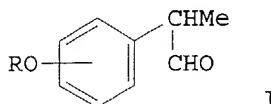
CLASSIFICATION: 25-15 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

Section cross-reference(s): 1

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63290837	A2	19881128	JP 1987-125683	19870525
PRIORITY APPLN. INFO.:			JP 1987-125683	19870525
OTHER SOURCE(S):		MARPAT 111:194298		
GRAPHIC IMAGE:				

**ABSTRACT:**

The title compds. I (R = Ph, Me), useful as drug intermediates, were prepared Dehydrogenation of 3-phenoxyphenylethane, followed by hydroformylation of the product in the presence of (Ph₃P)₃Rh(CO)H under H and CO, gave 2-(3-phenoxyphenyl)propionaldehyde with 91% selectivity and 99.1% conversion of 3-phenoxyphenylethane.

SUPPL. TERM: phenylpropionaldehyde prepn drug intermediate; fenoprofen intermediate phenylpropionaldehyde prepn; hydroformylation phenylethylene

INDEX TERM: Hydroformylation
(of phenylethylenes)

INDEX TERM: 17185-29-4, Hydridocarbonyltris(triphenylphosphine) rhodium
ROLE: CAT (Catalyst use); USES (Uses)

INDEX TERM: (catalyst, for hydroformylation of phenylethylenes)
1515-95-3 10568-38-4, 3-Methoxyphenylethane
36207-23-5, 4-Phenoxyphenylethane 78427-95-9,
3-Phenoxyphenylethane
ROLE: RCT (Reactant); RACT (Reactant or reagent)

INDEX TERM: (dehydrogenation of)
20401-88-1P 40138-66-7P 54954-44-8P 122801-83-6P
ROLE: SPN (Synthetic preparation); FORM (Formation,
nonpreparative); PREP (Preparation)

INDEX TERM: (formation of, in preparation of drug intermediate)
630-08-0
ROLE: RCT (Reactant); RACT (Reactant or reagent)

INDEX TERM: (hydroformylation, of phenylethylenes)
29679-58-1
ROLE: RCT (Reactant); RACT (Reactant or reagent)

INDEX TERM: (intermediates for, preparation of phenylpropionaldehydes as)
626-20-0P 637-69-4P, 4-Methoxyphenylethylene 4973-29-9P,
4-Phenoxyphenylethylene 63444-54-2P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)

INDEX TERM: (preparation and hydroformylation of)
5405-83-4P 59452-86-7P 59908-87-1P 80793-26-6P
123490-60-8P 123490-61-9P
ROLE: SPN (Synthetic preparation); PREP (Preparation)

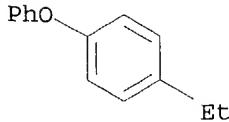
INDEX TERM: (preparation of, as drug intermediate)

IT 36207-23-5, 4-Phenoxyphenylethane
RL: RCT (Reactant); RACT (Reactant or reagent)

(dehydrogenation of)

RN 36207-23-5 HCPLUS

CN Benzene, 1-ethyl-4-phenoxy- (9CI) (CA INDEX NAME)



L24 ANSWER 9 OF 15 HCPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1987:17058 HCPLUS
 DOCUMENT NUMBER: 106:17058
 ENTRY DATE: Entered STN: 24 Jan 1987
 TITLE: Biotechnological preparation of optically active
 α -arylalkanoic acids
 INVENTOR(S): Cesti, Pietro; Piccardi, Paolo
 PATENT ASSIGNEE(S): Montedison S.p.A., Italy
 SOURCE: Eur. Pat. Appl., 11 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 INT. PATENT CLASSIF.:
 MAIN: C12P007-40
 SECONDARY: C12P017-14; C12P041-00
 CLASSIFICATION: 16-5 (Fermentation and Bioindustrial Chemistry)
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 195717	A2	19860924	EP 1986-400558	19860317
EP 195717	A3	19890222		
EP 195717	B1	19911009		
	R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE			
AT 68210	E	19911015	AT 1986-400558	19860317
US 4762793	A	19880809	US 1986-840856	19860318
JP 61239899	A2	19861025	JP 1986-61067	19860320
HU 41069	A2	19870330	HU 1986-1202	19860321
HU 197943	B	19890628		
ES 553215	A1	19870516	ES 1986-553215	19860321
PRIORITY APPLN. INFO.:			IT 1985-20036	19850322
			EP 1986-400558	19860317

OTHER SOURCE(S): CASREACT 106:17058

ABSTRACT:

S(T) α -arylalkanoic acids are efficiently obtained from racemic esters by using an esterase produced by a microorganism that is capable of asym. hydrolyzing the racemic ester, i.e. capable of selectively hydrolyzing the S(t) enantiomer, in order to yield an acid substantially in the S(t) form, while leaving the ester in the R(-) form unaltered. Thus, lipase from *Candida cylindracea* was reacted with the ethoxycarbomethyl ester of (R,S) 2-(4-isobutylphenyl)propionic acid for 24 h at 28° to yield the S(+) acid at a conversion rate of 45% equal to 90% hydrolysis of the S(+) form.

SUPPL. TERM: arylalkanoate asym hydrolysis esterase microorganism;
 carboxylate asym hydrolysis esterase
 INDEX TERM: Asymmetric synthesis and induction
 (arylalkanoic acid manufacture by, with lipase of *Candida cylindracea*)
 INDEX TERM: Microorganism
 (esterase of, arylalkanoic acid manufacture by asym.)

INDEX TERM: hydrolysis with)
Candida rugosa
 (lipase of, arylalkanoic acid manufacture by asym. hydrolysis
 with)

INDEX TERM: Carboxylic acids, preparation
 ROLE: BMF (Bioindustrial manufacture); BIOL (Biological
 study); PREP (Preparation)
 (aryl, manufacture of, by asym. hydrolysis with esterase of
 microorganisms)

INDEX TERM: 9013-79-0
 ROLE: BIOL (Biological study)
 (arylalkanoic acid manufacture by asym. hydrolysis with, of
 microorganism)

INDEX TERM: 9001-62-1, Lipase
 ROLE: BIO (Biological study)
 (arylalkanoic acid manufacture by asym. hydrolysis with, of
Candida cylindracea)

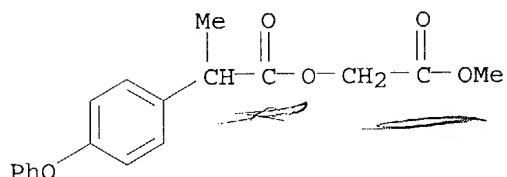
INDEX TERM: 64622-29-3 105052-65-1 105888-62-8 105888-63-9
 105888-65-1 105888-66-2 **105888-67-3**
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (asym. hydrolysis of, to arylalkanoic acid, with lipase
 of microorganisms)

INDEX TERM: 23981-80-8P 51146-56-6P 105888-60-6P 105888-64-0P
 105929-99-5P 105930-00-5P 105930-01-6P
105930-02-7P 105930-03-8P 105930-04-9P
 ROLE: BMF (Bioindustrial manufacture); BIOL (Biological
 study); PREP (Preparation)
 (manufacture of, by asym. hydrolysis with esterase of
 microorganisms)

IT **105888-67-3**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (asym. hydrolysis of, to arylalkanoic acid, with lipase of
 microorganisms)

RN 105888-67-3 HCPLUS

CN Benzeneacetic acid, α -methyl-4-phenoxy-, 2-methoxy-2-oxoethyl ester
 (9CI) (CA INDEX NAME)

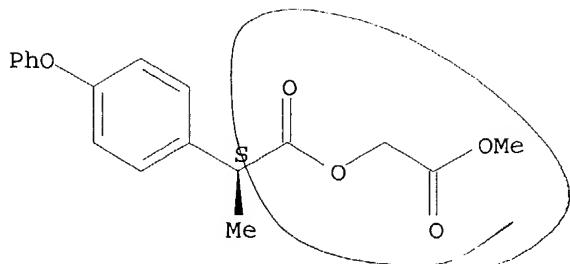


IT **105930-02-7P**
 RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP
 (Preparation)
 (manufacture of, by asym. hydrolysis with esterase of microorganisms)

RN 105930-02-7 HCPLUS

CN Benzeneacetic acid, α -methyl-4-phenoxy-, 2-methoxy-2-oxoethyl ester,
 (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 10 OF 15 HCPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1984:551531 HCPLUS
 DOCUMENT NUMBER: 101:151531
 ENTRY DATE: Entered STN: 27 Oct 1984
 TITLE: Thallium in organic synthesis. 62. A convenient synthesis of α -arylsuccinic acids
 AUTHOR(S): Taylor, Edward C.; Conley, Richard A.; Katz, Alan H.; McKillop, Alexander
 CORPORATE SOURCE: Dep. Chem., Princeton Univ., Princeton, NJ, 08544, USA
 SOURCE: Journal of Organic Chemistry (1984), 49(20), 3840-1
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 CLASSIFICATION: 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 OTHER SOURCE(S): CASREACT 101:151531

ABSTRACT:
 α -Arylsuccinic acids are readily prepared by oxidative rearrangement of β -arylpropionic acids (from arenes and succinic anhydride) with Tl(NO₃)₃-HC(OMe)₃. Application of the same reaction to β -benzoylbutyric acid, β -benzoylvaleric acid, 1,2-dibenzoylethane and 1,4-dibenzoylbutane gives di-Me α -phenylglutarate, di-Me α -phenyladipate, di-Me α, α' -diphenylsuccinate, and di-Me α, α' -diphenyladipate, resp. Oxidative rearrangement of unsym. 1,2-diaroylethanes gives unsym. di-Me α, α' -diarylsuccinates.

SUPPL. TERM: | benzoylelakanoic acid oxidative rearrangement; benzoylelakane di oxidative rearrangement; alkanoic acid benzoyl oxidative rearrangement; alkane dibenzoyl oxidative rearrangement; oxidative rearrangement dibenzoylalkane benzoylalkanoic acid; thallium nitrate oxidative rearrangement
 INDEX TERM: | Oxidation
 (rearrangement and, of benzoylelakanoic acids and dibenzoylalkanes with thallium trinitrate and tri-Me orthoformate, diesters by)
 INDEX TERM: | Rearrangement
 (oxidative, of benzoylelakanoic acids and dibenzoylalkanes with thallium trinitrate and tri-Me orthoformate, diesters by)
 INDEX TERM: 5447-74-5 25333-24-8 39560-31-1 57498-54-1
 67173-95-9 91266-23-8
 INDEX TERM: | ROLE: PROC (Process)
 (conversion of, to enol ether)
 INDEX TERM: 366-77-8 495-71-6 2051-95-8 3153-44-4 3375-38-0
 4144-62-1 4619-20-9 36330-86-6 51908-41-9 89229-73-2
 91266-20-5 91266-21-6 91266-22-7 91266-24-9
 91266-25-0 91266-26-1
 INDEX TERM: | ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (oxidative rearrangement of, with thallium trinitrate and

INDEX TERM: tri-Me orthoformate)
 1496-23-7P 10436-86-9P 15463-92-0P 22248-26-6P
 36265-44-8P 81631-72-3P **91266-19-2P**
 ROLE: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of by oxidative rearrangement of benzoylalkanoic acid with thallium trinitrate and tri-Me orthoformate)

INDEX TERM: 7300-04-1P 19020-59-8P 91280-66-9P
 ROLE: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by oxidative rearrangement of dibenzoylalkane with thallium nitrate and tri-Me orthoformate)

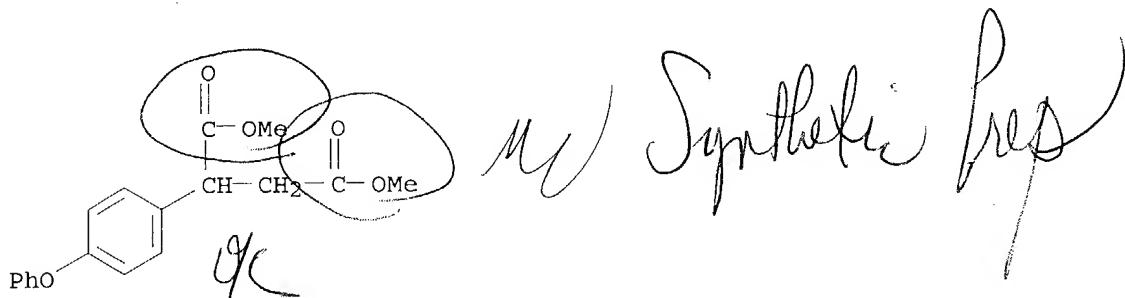
INDEX TERM: 149-73-5
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (thallium trinitrate and, oxidative rearrangement of benzoylalkanoic acids and dibenzoylalkanes by)

INDEX TERM: 13746-98-0
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (tri-Me orthoformate and, oxidative rearrangement of benzoylalkanoic acids and dibenzoylalkanes by)

IT **91266-19-2P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by oxidative rearrangement of benzoylalkanoic acid with thallium trinitrate and tri-Me orthoformate)

RN 91266-19-2 HCAPLUS

CN Butanedioic acid, (4-phenoxyphenyl)-, dimethyl ester (9CI) (CA INDEX NAME)



L24 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1977:467848 HCAPLUS
 DOCUMENT NUMBER: 87:67848
 ENTRY DATE: Entered STN: 12 May 1984
 TITLE: α -Aryl-substituted propionic acids
 INVENTOR(S): Takeda, Makoto; Uchide, Masayuka; Iwane, Hiroshi
 PATENT ASSIGNEE(S): Mitsubishi Petrochemical Co., Ltd., Japan
 SOURCE: Ger. Offen., 43 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 INT. PATENT CLASSIF.: C07C069-76
 CLASSIFICATION: 23-16 (Aliphatic Compounds)
 Section cross-reference(s): 25, 26
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

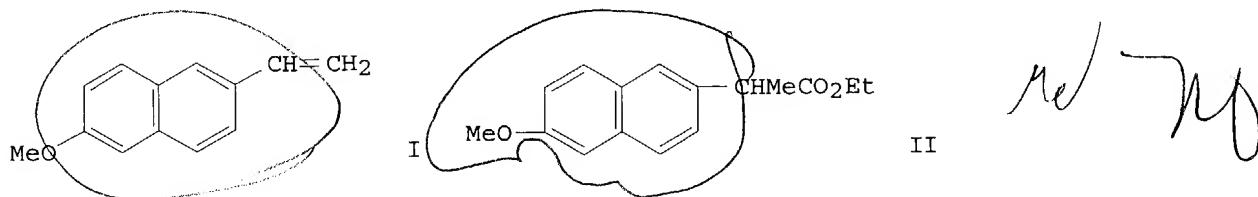
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2646792	A1	19770428	DE 1976-2646792	19761016
DE 2646792	C2	19850509		
JP 52051338	A2	19770425	JP 1975-127787	19751023

JP 59035899	B4	19840831		
JP 60045171	B4	19851008	JP 1976-91523	19760731
GB 1565235	A	19800416	GB 1976-43221	19761018
FR 2328689	A1	19770520	FR 1976-32143	19761025
FR 2328689	B1	19830121		
US 4329507	A	19820511	US 1980-111978	19800114
PRIORITY APPLN. INFO.:				
			JP 1975-127787	19751023
			JP 1976-91523	19760731
			US 1976-734592	19761021
			US 1978-909643	19780525

OTHER SOURCE(S):

CASREACT 87:67848

GRAPHIC IMAGE:



ABSTRACT:

Alkoxy carbonylation by alcs. and CO and carboxylation by H₂O and CO of vinylarenes were catalyzed by Pd complexes. Thus, I in EtOH containing (Ph₃P)₂PdCl₂, BF₃·Et₂O, and Ph₂NNO was autoclaved with CO to give 69% II.

SUPPL. TERM: alkoxy carbonylation vinylarene catalyst; carboxylation vinylarene catalyst; propionic acid aryl
 INDEX TERM: Alkoxy carbonylation catalysts
 (palladium complexes, for vinylarenes)
 INDEX TERM: 5338-96-5
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (Grignard reaction of)
 INDEX TERM: 391-08-2 716-89-2 3139-85-3 4973-29-9 10473-10-6
 30215-52-2 54314-33-9 63444-51-9 63444-52-0
 63444-53-1 63444-54-2 63444-55-3 63444-56-4
 63444-57-5
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (alkoxy carbonylation of)
 INDEX TERM: 109-63-7 603-35-0, uses and miscellaneous 7647-10-1
 13965-03-2 14977-08-3
 ROLE: CAT (Catalyst use); USES (Uses)
 (catalyst, for alkoxy carbonylation of vinylarenes)
 INDEX TERM: 62049-65-4
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (dehydrochlorination of)
 INDEX TERM: 5002-42-6 42771-85-7
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (hydride reduction of)
 INDEX TERM: 40150-92-3P 56430-69-4P 63444-59-7P
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (preparation and dehydration of)
 INDEX TERM: 56430-44-5P
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (preparation and dehydrohalogenation of)
 INDEX TERM: 37961-57-2P 41283-72-1P 61001-75-0P
 61566-34-5P 63444-58-6P

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and hydrolysis of)

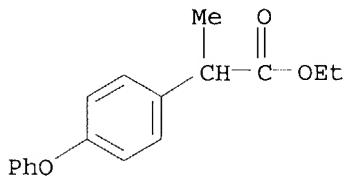
INDEX TERM: 3585-53-3P 5005-84-5P 6908-47-0P 15687-27-1P
 17692-38-5P 22410-97-5P 23981-80-8P 29679-58-1P
 36141-62-5P 36950-96-6P 41604-03-9P 51106-57-1P

ROLE: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

IT 61001-75-0P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and hydrolysis of)

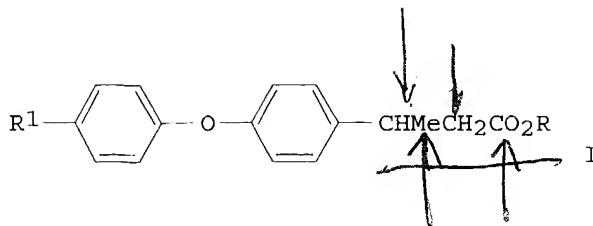
RN 61001-75-0 HCPLUS

CN Benzeneacetic acid, α -methyl-4-phenoxy-, ethyl ester (9CI) (CA INDEX NAME)



L24 ANSWER 12 OF 15 HCPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1976:592403 HCPLUS
 DOCUMENT NUMBER: 85:192403
 ENTRY DATE: Entered STN: 12 May 1984
 TITLE: Phenoxyphenylbutyric acid derivatives
 INVENTOR(S): Gante, Joachim; Kurmeier, Hans A.; Schacht, Erich;
 Mehrhof, Werner; Wild, Albrecht
 PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Fed. Rep. Ger.
 SOURCE: Ger. Offen., 51 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 INT. PATENT CLASSIF.: C07C069-76
 CLASSIFICATION: 25-18 (Noncondensed Aromatic Compounds)
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2509891	A1	19760923	DE 1975-2509891	19750307
SE 7602744	A	19760908	SE 1976-2744	19760227
AU 7611555	A1	19770908	AU 1976-11555	19760302
AU 497104	B2	19781130		
BE 839211	A2	19760906	BE 1976-7000789	19760304
FR 2302731	A1	19761001	FR 1976-6130	19760304
DK 7600979	A	19760908	DK 1976-979	19760305
NL 7602341	A	19760909	NL 1976-2341	19760305
ZA 7601340	A	19770223	ZA 1976-1340	19760305
ES 445793	A1	19770901	ES 1976-445793	19760305
GB 1494462	A	19771207	GB 1976-8980	19760305
AT 7601624	A	19790515	AT 1976-1624	19760305
JP 51125348	A2	19761101	JP 1976-25990	19760308
PRIORITY APPLN. INFO.:			DE 1975-2509891	19750307
GRAPHIC IMAGE:				



~~✓ Lamda~~

ABSTRACT:

The title compds. (I; R = H, Me, Et, Pr, Bu, tert-Bu, Et₂NCH₂CH₂, Me₂NCH₂CH₂; R₁ = H, Br, Cl, F), useful as analgesics and antipyretics, are prepared by a variety of standard procedures. Thus, reduction and hydrolysis of 4-(4-ClC₆H₄O)C₆H₄CMe(OH)CH₂CO₂Et with 67% aqueous HI in AcOH 1 hr at 150° gives I (R = H, R₁ = Cl).

SUPPL. TERM: phenoxyphenylbutyrate analgesic antipyretic; butyrate halophenoxyphenyl analgesic antipyretic

INDEX TERM: Analgesics
Antipyretics

INDEX TERM: 55102-99-3
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction with K 3-iodobutyrate)

INDEX TERM: 61001-87-4 61001-88-5
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction with carbon dioxide)

INDEX TERM: 78-09-1 124-38-9, reactions 541-41-3 61001-86-3
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction with halophenyl ethers)

INDEX TERM: 61001-75-0
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(chlorination of)

INDEX TERM: 61001-98-7
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(deamination and fluoroamination of)

INDEX TERM: 61001-97-6
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(deamination of)

INDEX TERM: 61001-90-9 61001-91-0
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(decarboxylation of)

INDEX TERM: 60467-98-3 61001-74-9
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation and hydrolysis of)

INDEX TERM: 61001-76-1 61024-36-0
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of)

INDEX TERM: 61001-89-6
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis and decarboxylation of)

INDEX TERM: 58727-42-7 58727-45-0
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis and reduction of)

INDEX TERM: 61001-78-3 61001-79-4 61001-80-7 61001-81-8
61001-82-9

INDEX TERM: 58727-63-2 61001-94-3
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of)

INDEX TERM: 58727-63-2 61001-94-3
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of)

INDEX TERM: 61001-57-8P 61001-61-4P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)

INDEX TERM: 61001-58-9P 61001-64-7P 61001-65-8P 61001-66-9P
61001-67-0P 61001-71-6P 61001-72-7P 61001-73-8P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

INDEX TERM: 61001-59-0P 61001-60-3P 61001-63-6P 61001-68-1P
61001-70-5P
ROLE: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

INDEX TERM: 1099-45-2
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction with 4-(1-bromoethyl)-4'-fluorodiphenyl ether)

INDEX TERM: 61024-35-9
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction with carbon monoxide)

INDEX TERM: 1951-12-8 7425-49-2
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction with chlorophenyl phenyl ether)

INDEX TERM: 61001-95-4
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction with diethylamine)

INDEX TERM: 352-34-1
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction with disodium 3-(4-hydroxyphenyl)butyrate)

INDEX TERM: 61001-77-2
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction with ethyl [triphenylphosphoranylidene]acetate)

INDEX TERM: 61001-83-0 61001-84-1
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction with ethyl bromobutyrate)

INDEX TERM: 61024-34-8
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction with fluoroiodobenzene)

INDEX TERM: 61001-93-2
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction with formic acid and with nickel carbonyl)

INDEX TERM: 7005-72-3
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction with halobutyrates)

INDEX TERM: 13463-39-3
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction with halophenyl ethers)

INDEX TERM: 61001-92-1
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction with nickel carbonyl)

INDEX TERM: 100-35-6 107-99-3
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction with sodium [(chlorophenoxy)phenyl]butyrate)

INDEX TERM: 61001-96-5
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction with sodium fluorophenolate)

INDEX TERM: 61001-85-2
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction with tert-butyl alc. and propanol)

INDEX TERM: 371-35-7
ROLE: RCT (Reactant); RACT (Reactant or reagent)

INDEX TERM: (reaction with sodium (iodophenyl)butyrate)
 64-18-6, reactions
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (with 4-chlorophenyl 4-(2-propenyl)phenyl ether)

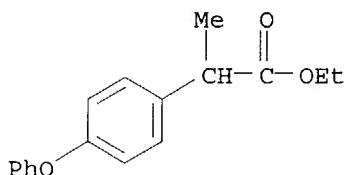
INDEX TERM: 630-08-0, reactions
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (with [(chlorophenoxy)phenyl]propanol)

INDEX TERM: 109-89-7, reactions
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (with chloroethyl [(chlorophenoxy)phenyl]butyrate)

IT 61001-75-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (chlorination of)

RN 61001-75-0 HCAPLUS

CN Benzeneacetic acid, α -methyl-4-phenoxy-, ethyl ester (9CI) (CA INDEX NAME)



L24 ANSWER 13 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1972:144751 HCAPLUS

DOCUMENT NUMBER: 76:144751

ENTRY DATE: Entered STN: 12 May 1984

TITLE: Effect of introducing ethyl radical to benzene derivatives on their odorant properties

AUTHOR(S): Wizner, Iwonna

CORPORATE SOURCE: Inst. Chem. Przem., Warsaw, Pol.

SOURCE: Tluszcze, Srodki Piorace, Kosmetyki (1971), 15(5), 20-30

DOCUMENT TYPE: CODEN: TSPKBZ; ISSN: 0372-1795

LANGUAGE: Journal

CLASSIFICATION: Polish

ABSTRACT: 62 (Essential Oils and Cosmetics)

ABSTRACT:

The effects of Et groups on odorant properties was studied in large number of esters, alcs., aldehydes, and ketones, as well as in p-ethyldiphenylmethane (I) and p-ethyldiphenyl ether. The most interesting scent was found in p-ethylacetophenone, I, Me p-ethylbenzoate, and p-ethylphenyl- β -butyl alc. Many of the compds. synthesized are not found in literature.

SUPPL. TERM: ethyl groups odorant; ester odorant ethyl effect; alc odorant ethyl effect; aldehyde odorant ethyl effect; ketone odorant ethyl effect

INDEX TERM: Molecular structure-property relationship
 (benzene ethyl derivs., odors)

INDEX TERM: Alcohols, properties

Aldehydes, properties

Esters, properties

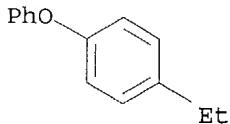
Ketones, properties

ROLE: PRP (Properties)

(odors of, ethyl radicals in relation to)

INDEX TERM: Odor and Odorous substances

(of benzene ethyl derivs.)
INDEX TERM: 768-59-2 4748-78-1 14062-20-5 22545-13-7 36207-03-1
36207-04-2 36207-05-3 36207-06-4 36207-07-5
36207-08-6 36207-09-7 36207-10-0 36207-13-3
36207-14-4 36207-15-5 36207-16-6 36207-18-8
36207-19-9 36305-78-9
ROLE: PRP (Properties)
(odor of)
INDEX TERM: 620-85-9 937-30-4 7364-20-7 36207-23-5
ROLE: PRP (Properties)
(odors of)
INDEX TERM: 36207-25-7P
ROLE: PREP (Preparation)
(preparation of)
IT 36207-23-5
RL: PRP (Properties)
(odors of)
RN 36207-23-5 HCPLUS
CN Benzene, 1-ethyl-4-phenoxy- (9CI) (CA INDEX NAME)



=> d ibib abs hitstr 13-
YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/ (N) :yn
YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/ (N) :n

=> d ibib abs hitstr 14-
YOU HAVE REQUESTED DATA FROM 2 ANSWERS - CONTINUE? Y/ (N) :y

L24 ANSWER 14 OF 15 USPATFULL on STN
ACCESSION NUMBER: 88:50260 USPATFULL
TITLE: Process for the biotechnological preparation of
optically active alpha-arylalkanoic acids
INVENTOR(S): Cesti, Pietro, Novara, Italy
Piccardi, Paolo, Milan, Italy
PATENT ASSIGNEE(S): Montedison S.p.A., Milan, Italy (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 4762793		19880809
APPLICATION INFO.:	US 1986-840856		19860318 (6)

	NUMBER	DATE
PRIORITY INFORMATION:	IT 1985-20036	19850322
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Rosen, Sam	
LEGAL REPRESENTATIVE:	Morgan & Finnegan	
NUMBER OF CLAIMS:	5	
EXEMPLARY CLAIM:	1	
LINE COUNT:	301	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB There is described the preparation of S(+) alpha-aryl-alkanoic acids by means of the reaction of a racemic ester(R,S) of the formula: ##STR1## wherein: R is a group selected from the group consisting of --C.tbd.CH, a --CH.dbd.CH.sub.2, --CN; --COCH.sub.3, --COO alkyl C.sub.1 C.sub.4 and --CH.sub.2 --O alkyl C.sub.1 -C4 group, Ar is a group selected from the group consisting of an aryl group and an aryl substituted or condensed with other groups, in particular a group selected from the group consisting of groups of the formula: ##STR2## wherein: R' is selected from the group consisting of C.sub.1 -C.sub.8 linear or branch of chain alkyl, C.sub.1 -C.sub.4 alkenyl, alkoxy, phenyl, phenoxy, tenoyl and heterocyclic;

R" is selected from the group consisting of hydrogen or halogen;

R'' is a C.sub.1 -C.sub.4 alkyl,

with an esterase, produced by microorganisms capable of selectively hydrolyzing the S(+) form of said racemic ester and by successively separating the S(+) acid from the unreacted ester.

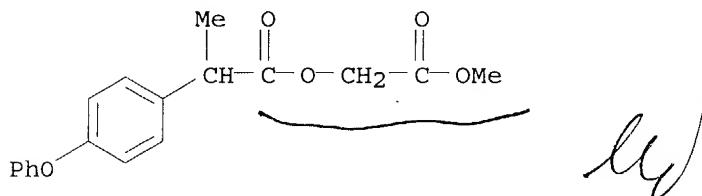
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 105888-67-3

(asym. hydrolysis of, to arylalkanoic acid, with lipase of microorganisms)

RN 105888-67-3 USPATFULL

CN Benzeneacetic acid, α -methyl-4-phenoxy-, 2-methoxy-2-oxoethyl ester (9CI) (CA INDEX NAME)



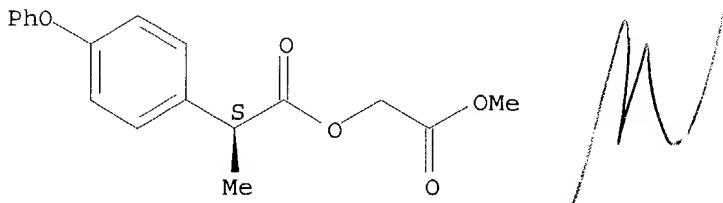
IT 105930-02-7P

(manufacture of, by asym. hydrolysis with esterase of microorganisms)

RN 105930-02-7 USPATFULL

CN Benzeneacetic acid, α -methyl-4-phenoxy-, 2-methoxy-2-oxoethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 15 OF 15 USPATFULL on STN

ACCESSION NUMBER: 82:22897 USPATFULL

TITLE: Substituted aryl ethylenes

INVENTOR(S): Takeda, Makoto, Amimachi, Japan

07/21/2004

PATENT ASSIGNEE(S):

Uchide, Masayuki, Amimachi, Japan
 Iwane, Hiroshi, Amimachi, Japan
 Mitsubishi Petrochemical Co., Ltd., Tokyo, Japan
 (non-U.S. corporation)

PATENT INFORMATION:

NUMBER	KIND	DATE
US 4329507		19820511
US 1980-111978		19800114 (6)

APPLICATION INFO.:

RELATED APPLN. INFO.: Division of Ser. No. US 1978-909643, filed on 25 May 1978, now abandoned which is a division of Ser. No. US 1976-734592, filed on 21 Oct 1976, now abandoned

PRIORITY INFORMATION:

NUMBER	DATE
JP 1975-127787	19751023
JP 1976-91523	19760731

DOCUMENT TYPE:

Utility

FILE SEGMENT:

Granted

PRIMARY EXAMINER:

Chan, Nicky

ASSISTANT EXAMINER:

Reamer, J. H.

LEGAL REPRESENTATIVE:

Burns, Robert E., Lobato, Emmanuel J., Adams, Bruce L.

NUMBER OF CLAIMS:

3

EXEMPLARY CLAIM:

1,2,3

LINE COUNT:

317

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

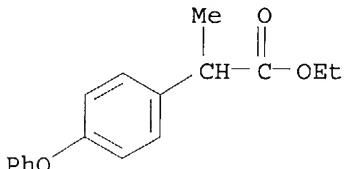
AB New substituted aryl ethylenes are disclosed which are produced by dehydration of the corresponding α - or β - (substituted aryl)ethyl alcohols or by dehydrohalogenation of the corresponding α - or β - (substituted aryl)ethyl halides.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 61001-75-0P

(preparation and hydrolysis of)

RN 61001-75-0 USPATFULL

CN Benzeneacetic acid, α -methyl-4-phenoxy-, ethyl ester (9CI) (CA INDEX NAME)

=>

*JL**Mopl!*